1984

Hydrocracking of Model Coal Derived Liquid Components Over a Zeolite Catalyst. (Volumes I and II) (Fluorene, Decalin).

William David Constant
Louisiana State University and Agricultural & Mechanical College

Constant, William David

HYDROCRACKING OF MODEL COAL DERIVED LIQUID COMPONENTS OVER A ZEOLITE CATALYST. (VOLUMES I AND II)

The Louisiana State University and Agricultural and Mechanical Col. PH.D. 1984

PLEASE NOTE:

In all cases this material has been filmed in the best possible way from the available copy. Problems encountered with this document have been identified here with a check mark __✓__.

1. Glossy photographs or pages _____
2. Colored illustrations, paper or print _____
3. Photographs with dark background _____
4. Illustrations are poor copy _____
5. Pages with black marks, not original copy _____
6. Print shows through as there is text on both sides of page _____
7. Indistinct, broken or small print on several pages ✓
8. Print exceeds margin requirements _____
9. Tightly bound copy with print lost in spine _____
10. Computer printout pages with indistinct print _____
11. Page(s) _____ lacking when material received, and not available from school or author.
12. Page(s) _____ seem to be missing in numbering only as text follows.
13. Two pages numbered 405. Text follows.
14. Curling and wrinkled pages _____
15. Dissertation contains pages with print at a slant, filmed as received _____
16. Other _____

_____

_____

University
Microfilms
International

HYDROCRACKING OF MODEL COAL DERIVED LIQUID COMPONENTS OVER A ZEOLITE CATALYST

VOLUME I

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

in

The Department of Chemical Engineering

by
William David Constant
B.S., Louisiana State University, 1977
M.S., Louisiana State University, 1980
August, 1984

Dedicated in memory of my father
Warren LeRoy Constant
whose inspiration gave me
the perseverance to complete
this work.

ACKNOWLEDGMENTS

Upon completion of this study, I welcome the opportunity to acknowledge with sincere appreciation the people who have made my stay in graduate school an enriching educational experience.

I was extremely fortunate to have had Dr. Edward McLaughlin as my major professor during the course of my graduate study. His encouragement, guidance, suggestions, and advice during this research and my graduate studies are greatly appreciated.

I would like to especially acknowlege my wife, Susan. Her love, understanding, and patience have provided me with an endless supply of moral support.

I would like to express my sincere thanks to the members of my examining committee, Dr. Douglas P. Harrison, Dr. Ralph W. Pike, and Dr. Geoffrey L. Price of the Department of Chemical Engineering, Dr. Zaki Bassiouni of the Department of Petroleum Engineering, and Dr. Leslie G. Butler of the Department of Chemistry, for their helpful suggestions and guidance.

A word of appreciation is due to the many people who have assisted me personally and/or professionally. Special thanks are extended to Dr. David M. Wetzel, Mrs. Jimmie Keebler, Miss Hazel LaCoste, Mr. Larry Veilleux and Mr. Steve Herron.

I appreciate the opportunity to teach on the collegiate level for two years and would like to acknowledge the Department of Chemical Engineering for affording me such an opportunity.

Financial support from the Exxon Company and the Department of Chemical Engineering is greatly appreciated. I sincerely appreciate the

suggestions and technical advice of Dr. Kenneth L. Riley of Exxon during this research.

Thanks are due to Mrs. Jan Easley for her skillful typing of the final manuscript.

Finally, I would like to extend my sincerest appreciation to my parents, for instilling in me at an early age the meaning of an education and for providing limitless encouragement and numerous forms of assistance throughout my life.

TABLE OF CONTENTS

VOLUME I

LIST OF TABLES

LIST OF FIGURES

ABSTRACT

Hydrocracking of fluorene was investigated over a nickel loaded Y zeolite in a fixed bed flow reactor using decalin as a donor solvent. This system served as a model for typical commercial donor solvent operations in order to develop a representative kinetic model and propose a reaction mechanism for refining of coal derived liquids.

After performing a qualitative investigation, base operating conditions of 661°K, 14.8 bar total pressure, 20 weight percent fluorene in decalin and a hydrogen to hydrocarbon ratio of 42 at a space-time of 4.8 seconds were established for the process. For each experimental series, the variable of interest was adjusted maintaining other conditions constant. Over the range of variables investigated, the effects of space-time and temperature were found to be most significant. No thermal reactions were observed during the study. The effect of hydrogen pressure was studied from 8.2 to 35.8 bar at 661°K, and no significant changes in the reaction occurred. Deactivation and coking were significant and the coke formation was found to be a function of catalyst exposure time. Deactivation was not included in the kinetic model as the route of coke formation was unknown.

Two kinetic models were developed using pseudo-homogeneous rate expressions of the chemistry as understood at this time. Rate coefficients were determined by numerical analysis of the experimental data and activation energies estimated. An overall reaction mechanism was proposed taking into account the roles of the donor solvent, catalyst, and hydrogen. It was proposed that decalin transferred hydrogen to fluorene adsorbed on the catalyst in a reactive state. The

cis-decalin isomer was highly reactive in isomerization, dehydrogenation, and cracking while trans-decalin was not as reactive. The kinetic model incorporates three routes for cracking of fluorene after partial hydrogenation from decalin; the side ring, the phenyl-methyl bond of the central ring, and both sides of the central ring.

Each component, decalin, nickel on the acidic catalyst, and hydrogen were found essential for hydrocracking of fluorene to occur. The product distribution was primarily benzenes, cyclopentanes, and C_2-C_6 hydrocarbon gases.

CHAPTER I.

Introduction

The conversion of coal to gasoline is a potential alternative to importing ever increasing amounts of crude petroleum in the near future. Only eleven percent of the world's estimated fossil fuel resources are oil and gas. Oil shale and tar sands account for about ten percent and the rest, nearly eighty percent, is coal. At present, coal contributes only about seventeen percent to our energy consumption. There are essential energy needs such as transportation which are almost entirely met by liquid fuels.

The production of oils and tars from coal predates the 20th century but it was not until the 1920's in Germany that there were serious efforts to develop technologies to produce liquid fuels from coal. Many of the coal liquefaction efforts today are based on that early work. Two approaches were developed, direct and indirect liquefaction. Indirect liquefaction involves gasifying coal to carbon monoxide and hydrogen and then synthesizing hydrocarbons from the gas. Processes by this method are already underway in South Africa. Direct liquefaction, on the other hand, involves the direct hydrogenation of coal to produce coal derived liquids as in Exxon's donor solvent process (E.D.S.).

Fundamental knowledge of coal chemistry is however, much less than we would expect from the length of time coal has been used. To begin with, the chemical structures of coal are complex and have been the subject of much discussion as have the structures of the coal liquids. In coal liquids condensed polynuclear aromatic compounds are the main component and may be difficult to process in the step after

liquefaction, the refining of the coal derived liquid. Several problems are encountered in this refining step over modern petroleum catalysts. Due to the presence of sulfur and nitrogen in the compounds, the catalyst may be poisoned. Hydrogen consumption by these aromatics is a factor of economic importance, also. The highly aromatic nature of coal derived liquids increases the chances of coking. Virtually all petroleum cracking and hydrocracking catalysts contain zeolites because of their exceptional activity, selectivity, and metal loading properties. However, when large polynuclear aromatic compounds are introduced, mass transfer limitations may exist.

At the present time, few details of the chemical reaction mechanisms of coal conversion and refining of coal derived liquids are known with certainty. A promising way to investigate these mechanisms is by studying the behavior of model coal derived liquid compounds. Although several model compounds have been investigated, one in particular, fluorene, has not been studied in a flow reactor with a donor solvent over a metal loaded zeolite at hydrocracking reaction conditions. This type of system would serve as a model for present commercial hydrocracking reactors and allows a detailed study to be performed.

The objective of this research is to investigate the reaction of this model polynuclear aromatic (fluorene) with emphasis on central ring cracking. With the use of a hydrogen donor solvent this can be performed in a flow reactor wherein product yield will be maximized and hydrogen consumption will be at a minimum. The fixed catalyst bed flow reactor used in this study allows for investigation of the reaction over a range of temperature, pressure, and concentrations. Previous

petroleum liquid studies with this experimental system are used as a basis for operating conditions. Sought as products are relatively low boiling paraffinic and naphthenic hydrocarbons and benzene, toluene, and xylenes which are typical of high octane fuel stocks.

In order to gain insight into the refining of coal derived liquid compounds, the specific objectives with respect to flourene hydrocracking with a donor solvent in hydrogen on a metal loaded zeolite catalyst are:

1. Development of an experimental system to obtain optimum processing conditions for hydrocracking of fluorene.

2. Study synergistic effects - the role of catalyst sites, molecular hydrogen, and the donor solvent.

3. Evaluate the catalyst for deactivation, coking, and diffusion limitations.

4. Propose a kinetic model and a reaction mechanism.

CHAPTER II.

Literature Review

1) The Process

Optimum future use of chemical resources will require a greatly increased role for coal. Coal has become a resource of great abundance that can be converted to gaseous and liquid fuels. As premium materials are depleted, attention is shifting to heavier materials, with coal, as presented by Haggin (1982a), being the extreme example. Cummings (1948) discussed the early work of the Germans in World War II, where out of necessity, they had to put considerable reliance on their oil from coal process, the feasibility of which had only been proven at that time and was known to be expensive and technically difficult. Considerable research is currently underway to develop economically competitive processes for the conversion of coal to liquid fuels. Patzer et al. (1979) reviewed this work using as examples several processes which use a catalyst, viz. SRC, EDS, Consol, Synthoil, H-Coal, and the Gulf process. However, Berg et al. (1982) reviewed these processes and noted that three have emerged as primary topics in the United States. They are Pittsburgh and Midway Coal Mining Co.'s SRC (solvent refined coal) process, Hydrocarbon Research, Inc.'s H-Coal process, and Exxon's donor solvent process (EDS).

Coal liquefaction processes generally involve a number of mechanical and chemical steps to bring about liquefaction. In a catalytic process, an important step is the catalytic hydrocracking of the coal liquid. The catalyst is believed to bring about the conversion of various molecules present to solvent molecules capable of

depolymerizing coal particles by hydrogen transfer (Furlong et al., 1976). There are two methods of coal liquefaction, the first is commonly refered to as the direct method, whereby coal is first extracted with solvent and the extract hydrogenated. This method was pioneered by Bergius (1913) in Germany. The second is the indirect method in which the coal is first gasified entirely with oxygen and steam to synthesis gas (carbon monoxide and hydrogen) and this mixture is then "reconstituted" to give hydrocarbons and alcohols by using different catalysts. This indirect method was discovered by Fischer and Tropsch (1925) and is now used in the SASOL plant in South Africa, which is the only commercial coal liquefaction plant in operation today. The war time hydrogenation of coal and coal tar as commercial projects ceased to exist after 1945, since it was not competitive with natural petroleum. However, extensive development efforts are now underway in many countries to provide a basis for a new and improved commercial coal liquefaction industry.

The research presented here is concerned with the production of gasoline from coal. Six industrial processes currently under study which produce gasoline and other fuels are summarized below for comparison (from Nowacki, 1979, Owen, 1981, Gallagher et al., 1979, and Brunson, 1979).

a) The Fischer-Tropsch (F.-T.) process begins with complete gasification of coal. Fixed bed catalytic reactors cause reaction of the feed gas to form a wide range of hydrocarbons and oxygenated hydrocarbon products. For production of the synthesis gas, the Lurgi coal gasification process was chosen. The commercial SASOL plant was designed to produce liquid hydrocarbons for motor fuels via the F.-T.

process. However, the product mixture is quite complex and many of them are undesirable for fuels as shown in Figure 2.1.

b) Mobil's M-Gasoline process has been tested in a pilot plant which treats 7.361×10^{-6} m^3/s (4 barrels/day) of crude methanol that is converted to 2.760×10^{-6} m^3/s (1.5 barrels/day) of 96 RON gasoline (Research Octane Number, representing moderate operating conditions), 4.600×10^{-6} m^3/s (2.5 barrels/day) of water, and fuel gas.

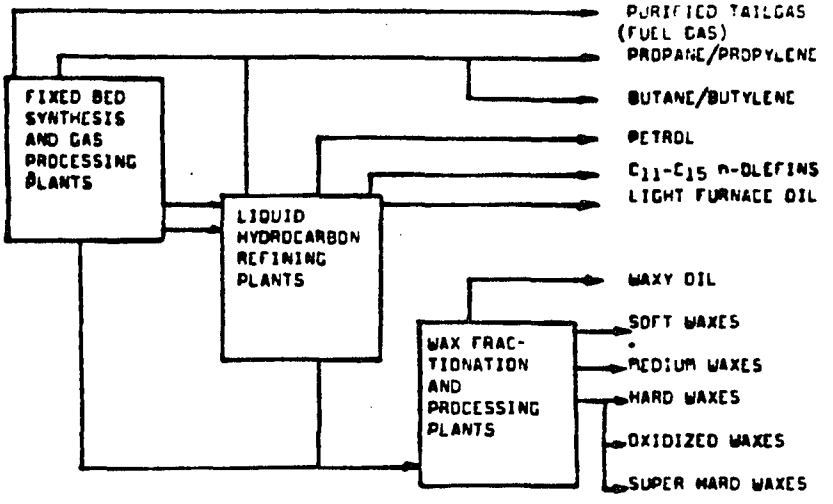
c) In the H-Coal process, dry ground coal in oil and hydrogen are fed to an ebullating bed catalytic reactor with treatment at 728°K and 208 bars. This pressure and temperature severity may be varied to favor production of either syncrude or a fuel oil with low quality naphtha in either case. The product is similar to that formed by the SRC process.

d) The solvent refined coal (SRC) process, developed by the Pittsburgh and Midway Coal Co., is a noncatalytic, hydrogenative, solvent treating process. The hydrogen is injected into the solvent as a gaseous phase and production may be operated in either a liquid or solid mode. The crushed coal is treated with a coal derived recycle solvent and hydrogen at 700°K and 70 bars. The liquid is known as SRC-II and the solid as SRC-I. Both are potential health hazards due to the presence of carcinogenic compounds and therefore are difficult to handle.

e) The Char-Oil-Energy Development (COED) process is based on four stage fludized bed pyrolysis of coal to produce oil, gas, and char. This pyrolysis is followed by catalytic hydrogenation of the liquid.

f) The Exxon donor solvent (EDS) process is similar to SRC except for the solvent used. It is a special coal-oil base solvent used to dissolve the coal and to contribute hydrogen to increase the hydrogen to

Fixed Bed Product Recovery Flow Diagram



Synthol Product Recovery Flow Diagram

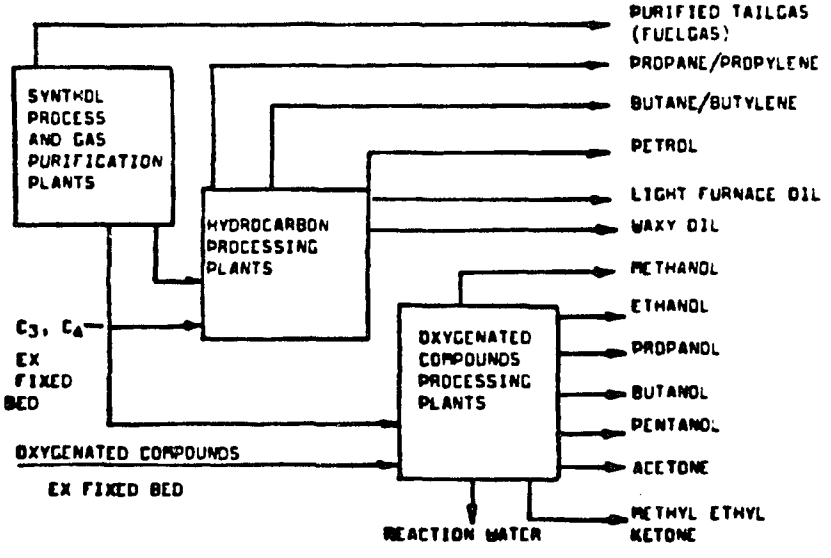


FIGURE 2.1 Products from Fischer-Tropsch Process (Nowacki, 1979).

carbon ratio in the products. The recycled solvent is hydrotreated on a continuous basis and it carries the crushed coal into a catalytic, fixed bed hydrogenation reactor as shown in Figure 2.2 as a simplified diagram from Brunson (1979). The donor vehicle serves a dual purpose as it dissolves coal and also provides hydrogen. The donor vehicle boiling range material is regenerated in a trickle bed of commercial hydrogenation catalyst prior to recycle. The EDS process is one of direct liquefaction and was chosen by Exxon as it was expected to be more thermally efficient and lower in cost than indirect liquefaction in the long term (Vick and Epperly, 1982).

The brief review of these six processes indicates that many routes are possible in making liquid fuels from coal. At this time it appears that EDS, SRC, and H-Coal processes yield relatively high amounts of desirable liquid products and for this reason are attractive for this research. Several conclusions may be drawn. Focusing on the EDS process, two steps are required, the first being liquefaction of the coal and secondly refining of the coal derived liquid (CDL). Obviously, much emphasis is presently being put on the difficult process of liquefaction with little work currently underway on the refining operation which may be equally difficult and important. Distillation of CDL's into light naphtha, middle distillate, and residuum oil yields fractions with substantial amounts of molecules containing three to nine condensed aromatic rings, sometimes highly substituted with naphthenes and paraffins. This reflects the essentially graphitic/aromatic structure of most coals. These large aromatic structures may be refined into usable fuels by employing hydrocracking as summarized by Satterfield (1980). Hydrocracking is a combination of catalytic

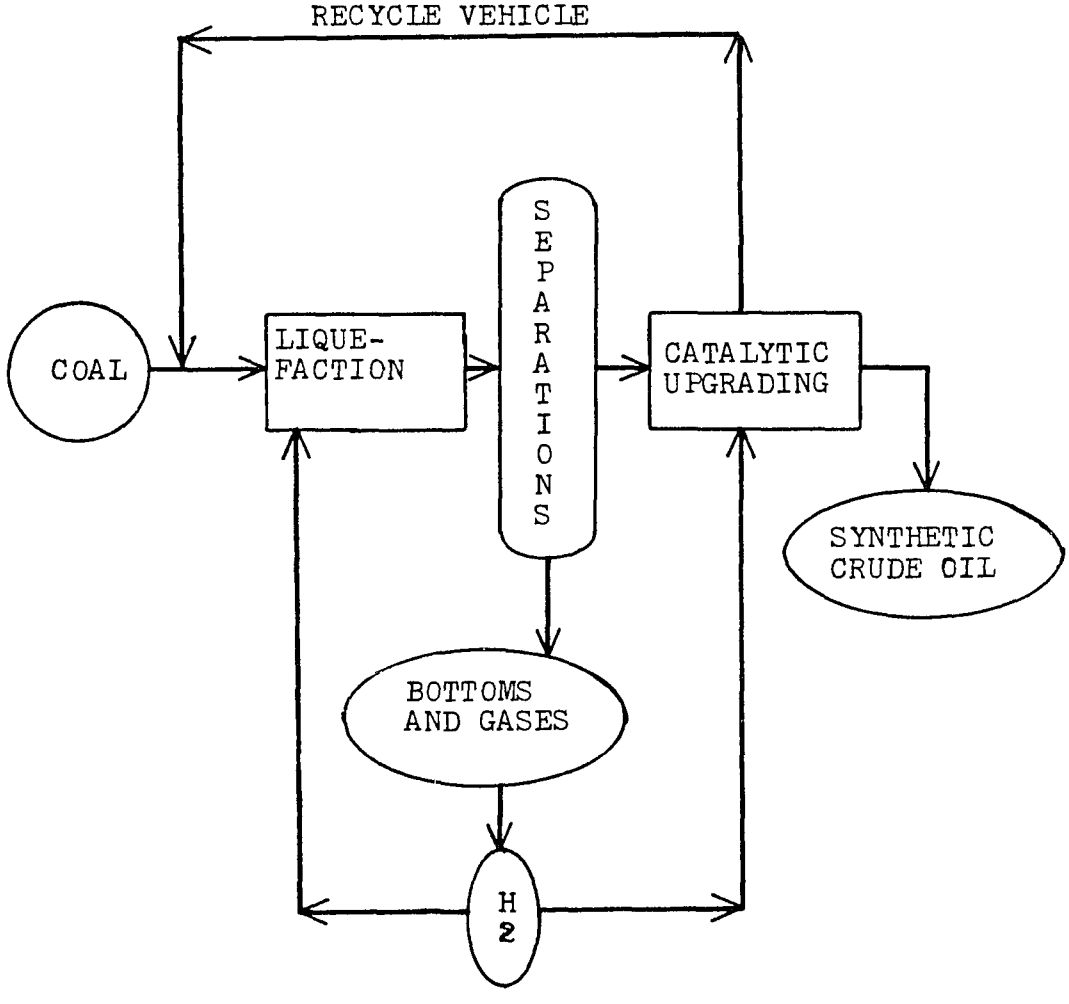


FIGURE 2.2 Simplified Diagram of EDS Process (Brunson, 1979).

cracking and hydrogenation under pressure. This process was developed for the petroleum industry to refine feeds with a high content of polycyclic aromatics, like those in coal liquids. Temperature is usually in the range of 472 to 672°K with hydrogen pressure from 11.35 to 104.4 bars. Catalysts must be dual functional, i.e., be able to crack the C-C bonds and also provide hydrogenation activity to "heal" the bonds. Highly active metal loaded zeolite catalysts have been found desirable for this process.

2) Coal and Related Compound Structure

Solomon (1981) found that although coal has been in use for over six hundred years, there is still no agreed upon model for the chemical structure or how it comes apart during a chemical reaction. As work continues in the processes previously discussed, it is imperative to obtain an understanding of the fundamental chemistry involved in both liquefaction of coal and the refining of coal derived liquids. Most accepted models concerning the structure of coal treat it as a highly condensed polynuclear aromatic substance made of fused aromatic and hydroaromatic ring clusters, possibly linked by relatively weak aliphatic bridges. The ring clusters contain heteroatoms (oxygen, sulfur, and nitrogen) and have a variety of attached functional groups.

Several investigators have suggested coal structures based on constraints provided by available data. Solomon (1981) summarizes much of this work and based on that information, formed a hypothetical coal molecule shown in Figure 2.3. His proposed structure is then cracked during thermal decomposition to yield fragments as shown in Figure 2.4. Further breakdown will yield coal-liquid type fragments. The size of

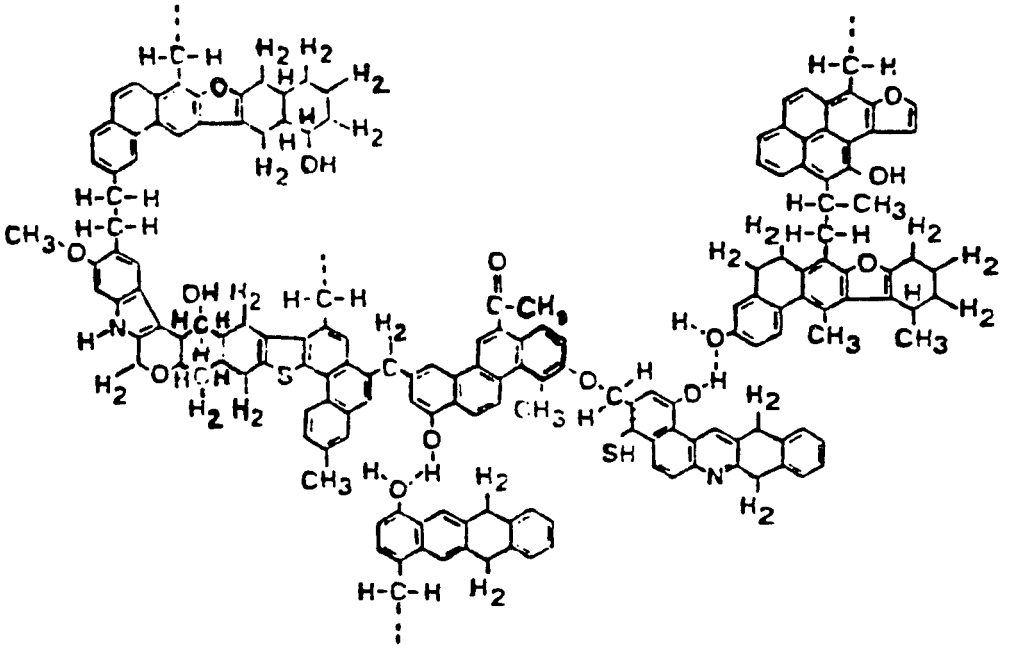


FIGURE 2.3 Hypothetical Coal Molecule (Solomon, 1981).

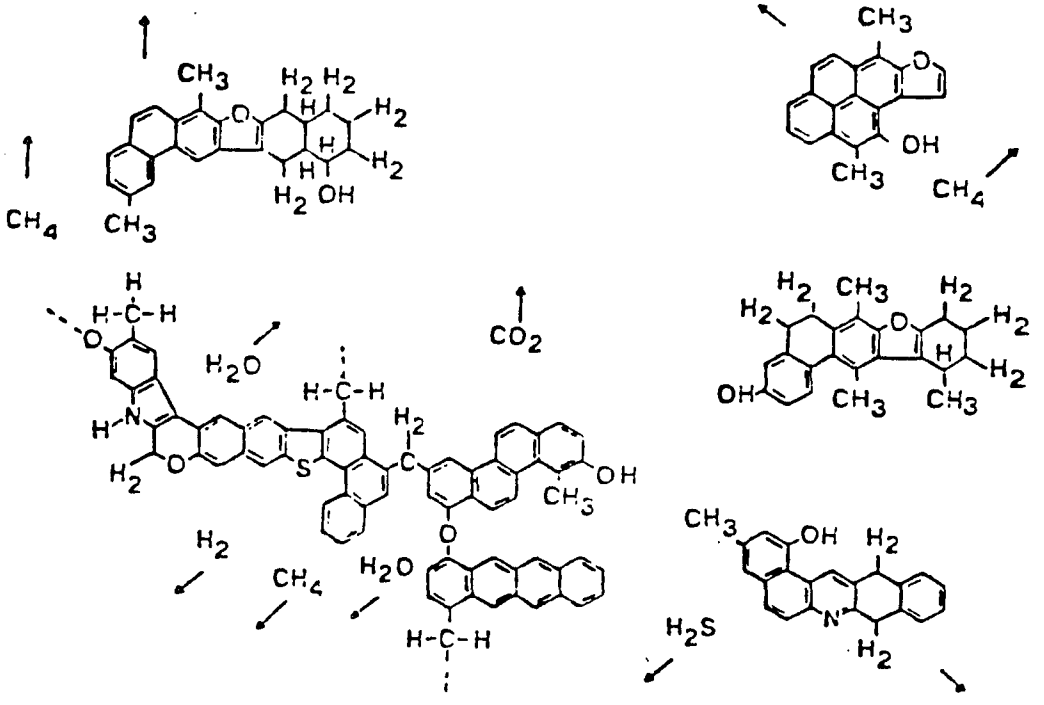
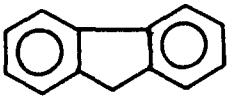


FIGURE 2.4 Cracking of Hypothetical Coal Molecule During Thermal Decomposition (Solomon, 1981).

these fragments may vary from one to several rings with typical compounds containing three or four rings. Bartle and Zander (1983) presented structures found in extracts of bituminous coals and lignite after extensive characterization work using chromatographic separation, NMR spectroscopy, mass spectroscopy, and electrochemical analysis. This work, summarized in Table 2.1, brings out two important points. First, the structures are similar to those in Figures 2.3 and 2.4 and secondly, a key structure in both examples is fluorene without functional groups or heteroatoms. As listed by Weast (1973), fluorene (2,3-benzindene or diphenylene methane) has a molecular weight of 166.23, a melting point of 389°K, boiling point of 567°K, and a density of 1203 kg/m^3 at 273.15°K. Its structure may be represented as:



which is similar to several of the polycyclic aromatic hydrocarbons shown in Figure 2.5. The higher members of the aromatic series are solid at room temperature as is fluorene. In working with a high melting point compound like fluorene, as in the handling of coal and its heavier constituents, it is necessary to have a proper solvent. In practice, the donor vehicle (solvent) is a recycle mixture of coal derived liquids as was shown for the EDS process. The concept of a donor vehicle is idealized by tetrahydronaphthalene (tetralin) wherein the aromatic portion dissolves coal and the saturated ring is a source of hydrogen. However, if solubility of fluorene is high enough, decahydronaphthalene (decalin) may prove to be an excellent donor vehicle. Decalin is represented as:

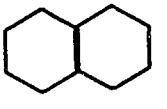
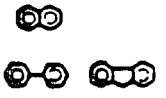
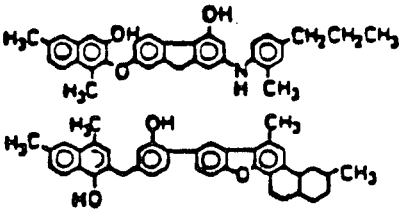
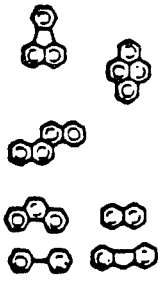
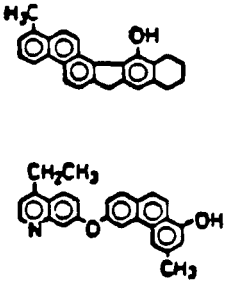
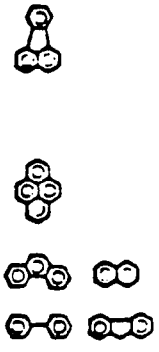
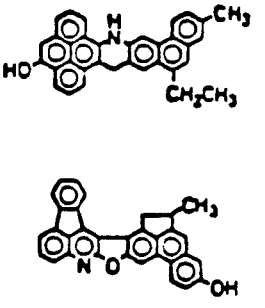
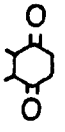
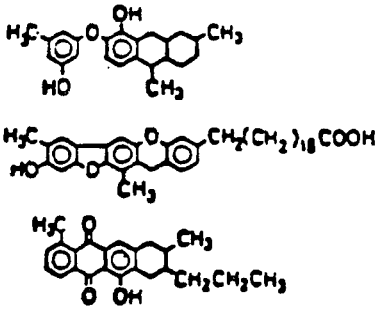


TABLE 2.1 Structures Identified by Voltammetry and NMR in Asphaltenes from SCG, HDS and Anthracene Oil Extracts (Bartle and Zander, 1983).

	Structure	NMR Average structures
Bituminous coal A SCG extract asphaltenes		
Bituminous coal A HDS extract asphaltenes		
Bituminous coal B Anthracene oil extract		
Lignite C SCG extract		

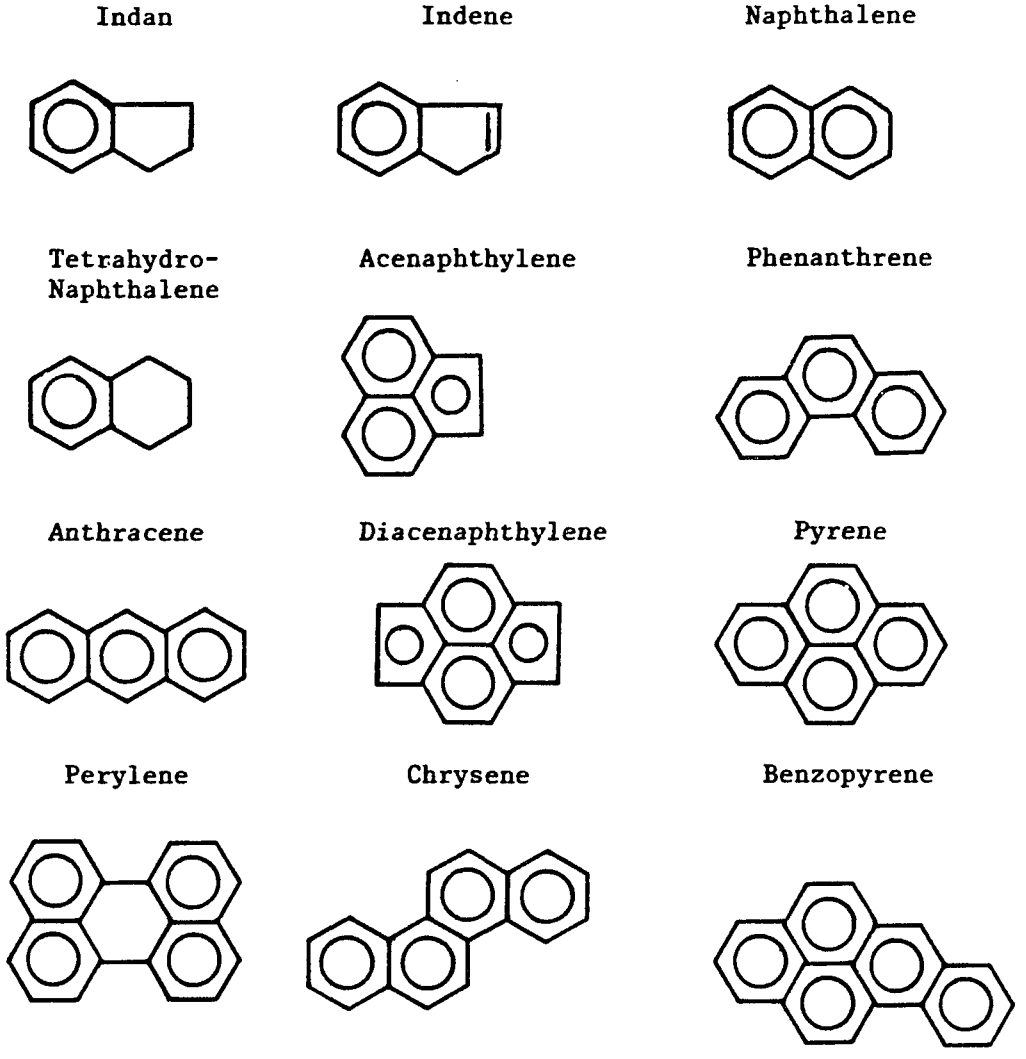


FIGURE 2.5 Polycyclic Aromatic Hydrocarbon Examples (Cusamano et al., 1978).

with a molecular weight of 138.25, a melting point of 230.15°K, a boiling point of 468.81°K, and a density of 896.5 kg/m^3 at 273.15°K for the cis- isomer. The trans- isomer has a melting point of 242.76°K, a boiling point of 460.41°K and a density of 869.9 kg/m^3 at 273.15°K. Unlike tetralin, decalin may exist in cis- or trans- forms with the cis- form in four different conformations and the trans- form three. This, as explained by Smith (1957), depends on whether the rings are in the chair or boat forms and whether the ring fusion involves polar or equatorial bonds.

With fluorene representing a coal liquid and decalin as a donor vehicle, two routes may exist in producing the primary products for motor gasoline with high octane numbers: the low boiling branched chain paraffins and benzene, toluene, and xylenes. Wiser et al. (1970) proposed the following general schemes which when applied to fluorene are as follows. The first route would consist of hydrogenation of a terminal ring followed by ring opening and cracking. The second route would be cracking of the central ring yielding benzene and toluene. In either case, hydrogen from decalin dehydrogenation would reduce molecular hydrogen consumption which must be kept to a minimum for economic reasons. With these large structures, as critical diameters listed in Table 2.2 indicate, it is also essential to have wide pore catalysts, and control over the hydrogenation/dehydrogenation to cracking ratio. Therefore, catalyst selection is critical.

3) Zeolite Catalyst Properties

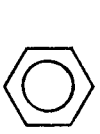
i) Basic Structures

Zeolites, crystalline aluminosilicate minerals, consist mainly of silicon, aluminum, and oxygen together with 10 to 20 percent water.

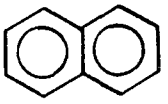
TABLE 2.2 Approximate Critical Diameters

Molecule	Critical diameter/Å
benzene	6.7
naphthalene	7.3
phenanthrene	7.9
pyrene	9.0
coronene	11.4
fluorene	7.5 (estimated)

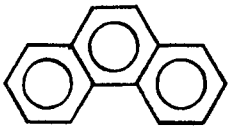
Calculation based on molecule being planar with bond lengths of C-C = 1.395 Å, C-H = 1.084 Å, and radius of H atom = 1.2 Å. (Unpublished research proposal, Haynes, H.W., Jr., 1977).



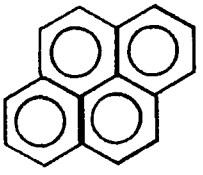
benzene



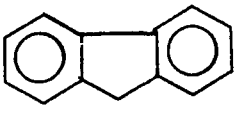
naphthalene



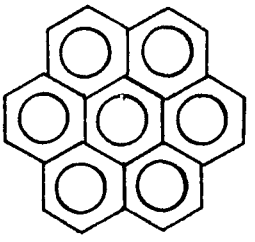
phenanthrene



pyrene



fluorene



coronene

Structures of molecules listed above.

Natural zeolites, which have been observed in many colors, decompose rapidly upon treatment with acid yielding a gelatinous mass. These minerals were recognized for their ability to exchange their metal cations by treatment with aqueous salt solutions. Early work on the sorptive properties of zeolites was summarized by McBain (1932) who proposed the name "molecular sieve". Since zeolites are crystalline in nature, their bulk properties are susceptible to study with techniques like X-ray diffraction (Gates et al., 1979). Zeolites generally used in hydrocracking (catalytic cracking with hydrogenation) are of the X and Y form of molecular sieves, wherein most of the sodium has been ion exchanged with ammonium ions, rare earth ions, etc. (Venuto and Habib, 1978). There are 34 known natural zeolites and about 100 without natural counterparts that have been synthesized (Gates et al., 1979).

All zeolites, natural and synthetic, may be represented by the empirical formula from Breck (1964):

$$Me_{x/n}\,[(AlO_2)_x\,(SiO_2)_y] * M\,H_2O$$

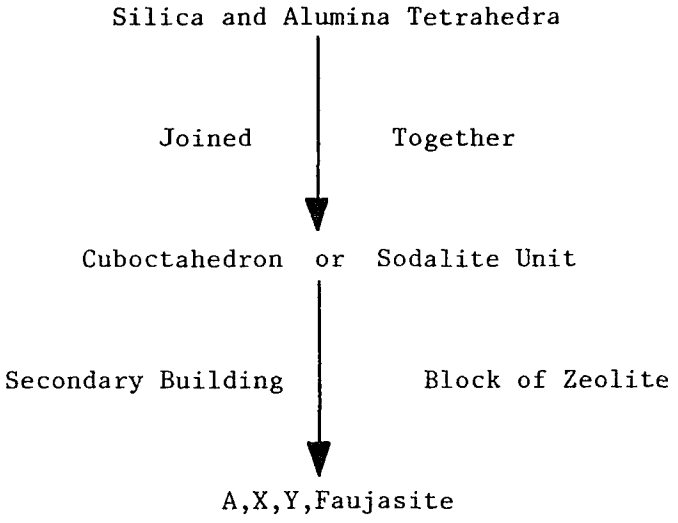
where "Me" represents a metal cation of valence "n" and "M" is the number of water molecules. The number of water molecules associated with one unit cell can vary over a range of at least 15 to 264. The Si/Al or Y/X ratio for the empirical formula ranges from unity for zeolite type A to a value of 5 for mordenite. Table 2.3 from Haggin (1982b) lists as examples several natural and synthetic zeolites used in the chemical industry.

The fundamental building block is a tetrahedron of 4 oxygen anions surrouding a smaller Si or Al ion. The alumina tetrahedron requires a +1 charge from a cation in the structure to maintain electrical neutrality. This is where a sodium ion or its ion exchange counterpart

TABLE 2.3 Natural and Synthetic Zeolite Compositions. (Haggin, 1982b).

Material	Typical composition	Crystalline form
Natural materials		
Cancrinite	$Na_6Al_6Sl_6O_{24}$-$CaCO_3$-$2H_2O$	Hexagonal
Chabazite	$(Ca,Na_2)_{\sim 2}Al_4Si_8O_{24}\cdot 13H_2O$	Rhombohedral
Erionite	$(Ca,K_2,Na_2)_4Al_8Si_{28}O_{72}\cdot 27H_2O$	Hexagonal
Faujasite	$\sim Na_{13}Ca_{11}Mg_9K_2Al_{55}Si_{137}O_{384}\cdot 235H_2O$	Isometric
Gmelinite	$(Na, etc.)_{\sim 8}Al_8Si_{18}O_{48}\cdot 24H_2O$	Hexagonal
Mazzite	$K_{2.5}Mg_{2.1}Ca_{1.4}Na_{0.3}Al_{10}Si_{28}O_{72}\cdot 28H_2O$	Hexagonal
Mordenite	$Na_8Al_8Si_{40}O_{96}\cdot 24H_2O$	Orthorhombic
Offertite	$KCaMgAl_5Si_{13}O_{36}\cdot 15H_2O$	Hexagonal
Sodalite	$Na_6Al_6Si_6O_{24}\cdot 2NaCl$	Isometric
Synthetic materials (dominant)		
Type-A	$Na_{12}Al_{12}Si_{12}O_{48}\cdot 27H_2O$	Isometric
Type-X	$Na_{86}Al_{86}Si_{106}O_{384}\cdot 264H_2O$	Isometric
Type-Y	$Na_{56}Al_{56}Si_{136}O_{384}\cdot 250H_2O$	Isometric
Type-L	$K_9Al_9Si_{27}O_{72}\cdot 22H_2O$	Hexagonal
Type-Ω	$(Na, etc.)_8Al_8Si_{28}O_{72}\cdot 21H_2O$	Hexagonal
Type-ZK5	$Na_{30}Al_{30}Si_{66}O_{192}\cdot 98H_2O$	Isometric
Type-ZMS5	$M_xAl_{1.1}Si_{94.9}O_{192}$ (anhydrous)	Orthorthombic (?)

fits into the structure. The following may be considered as a "construction scheme" for zeolites:

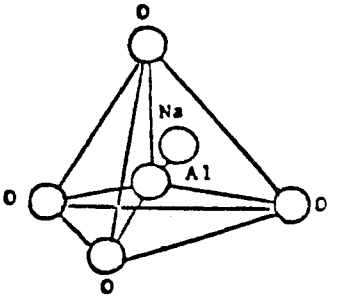


Depending on how the truncated octahedra are connected determines the type of zeolite formed and the resulting free pore aperture it contains. Gates et al. (1979) gave examples of the free pore aperture of various forms as listed in Table 2.4 for comparison to molecular critical diameters in Table 2.2. Figure 2.6 shows the arrangement of the basic building block tetrahedra, the sodalite structure, and the resulting forms of zeolite A and faujasite (type X and Y zeolites) structures. These representations show the differences in cage construction and relative aperture size.

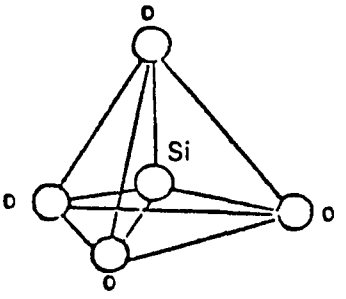
Zeolites possess selectivity and activity characteristics when processing petroleum fractions which are far superior to the older amorphous silica-alumina cracking catalysts. As shown in Table 2.5, from Miale et al. (1966), up to a 10,000 fold increase in activity may be accomplished relative to the activity of silica-alumina at 813.15°K. It is also important to note the low sodium concentration in the more

TABLE 2.4 Catalyst Structure Apertures (Gates et al. 1979).

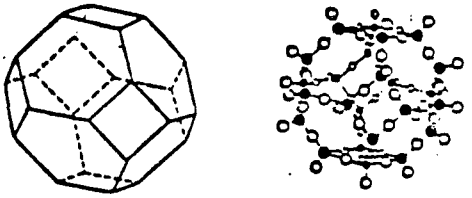
Catalyst Structure	Free Pore Aperture/Å
Sodalite	2.6
Zeolite A	4.2
Faujasite	7.4



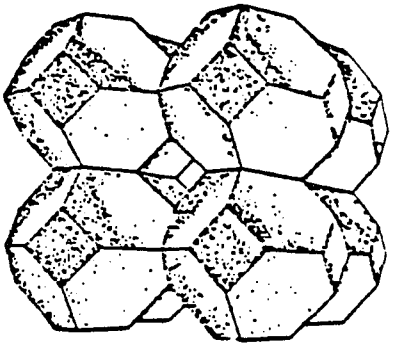
AlO_4 tetrahedron with monovalent sodium atom to balance charge



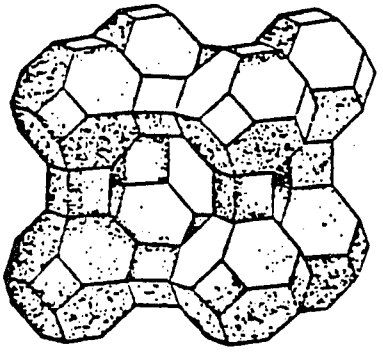
Electrically neutral SiO_4 tetrahedron



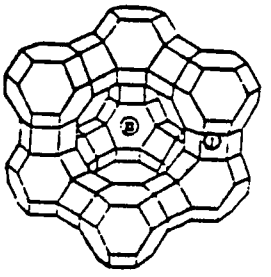
O - oxygen ● - Al or Si
Sodalite Cage Structure



Arrangement of truncated octahedra in sodalite



Arrangement of truncated octahedra in zeolite A



Faujasite structure
Type X and Y zeolites

FIGURE 2.6 Representations of Structures of Zeolites (adapted from Gates et al., 1979).

TABLE 2.5 Catalytic Activity of Various Zeolites (Miale et al., 1966)

Catalyst	Major cations exchanged into zeolite	Analysis of zeolite, wt%					Activity[a]	
		SiO_2	Al_2O_3	Na	Ca	RE	T/°K	α[b]
Amorphous SiO_1-Al_2O_3 (standard catalyst)		...	...	...	...	...	813	1.0
Faujasite	Ca^{2+}	47.8	31.5	7.7	12.3	...	803	1.1
	NH_4^+	75.7	23.1	0.4	...	...	623	6,400
	La^{3+}	...	...	0.4	...	29.0	543	7,000
	RE	...	...	0.39	...	28.8	<543	> 10,000
	RE, NH_4^+	40.0	33.0	0.22	...	26.5	<543	> 10,000
	RE, NH_4^+	...	...	...	...	...	693	20
Zeolite A	Ca^{2+}	42.5	37.4	7.85	13.0	...	833	0.6
Zeolite ZK5	...	...	...	...	...	...	673	38
	H^+	76.8	23.1	0.47	...	...	613	450
Mordenite	Ca^{2+}	(~77)	...	1.01	...	...	793	1.8
	Ca^{2+}, H^+	82.0	14.0	0.4	...	...	633-673	40-200
	NH_4^+	...	...	...	...	...	<543	> 10,000
	H^+	80.1	13.4	0.3	1.54	...	573	2,500
	NH_4^+	...	...	0.1	...	...	<543	> 10,000

a - Temperature required to achieve 5 to 20% conversion of n-hexane.

b - Activity of zeolite extrapolated to 813°K divided by the activity of silica-alumina at 813°K.

active zeolites. These have had cations exchanged into them and hence are more active (Venuto and Habib, 1978).

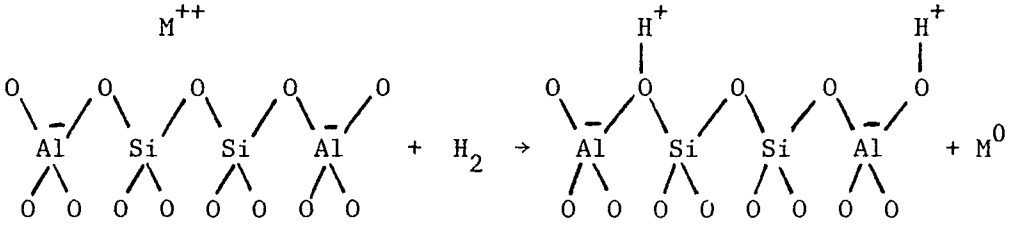
The discussion to follow will be concerned only with the large pore zeolites thereby omitting the molecular sieve or shape selective property explained by Chen and Weisz (1967). With large apertures, a wide variety of organic molecules may enter the structure. However there is a limit as observed by Riesz and Weber (1964) in the hydrogenation of soybean oil, where large and complex fat molecules are involved that size selectivity plays an important role. Catalysts containing the faujasite type structure have thus far achieved the greatest success of all the zeolites with respect to commercial applications. They have also been extensively studied so information concerning preparation, structure, nature of sites, etc. are available. Although preparation itself, which is part art and part science, is quite important, it will not be dealt with in detail as the zeolite base for this study is commercially available.

ii) Catalysts of Faujasite Structure

Hydrocracking of the aromatic structures of coal liquids requires the use of dual functional catalysts having both cracking and hydrogenation activity. The cracking activity is provided by the acidic support while hydrogenation (or dehydrogenation) is supplied by certain metals on the support. These metals are mostly from Groups VIB and VIII of the periodic table. One of the most widely used systems is nickel dispersed on various acidic supports.

Zeolite Y, a synthetic aluminosilicate, has a framework structure essentially the same as that of the naturally occuring, but rare mineral

faujasite. According to Break (1964a), the 3-D framework encompasses the supercages which are elliptical shaped cavities approximately 13Å in diameter. The supercages are entered through a 12 membered ring opening approximately 8Å in diameter. This large opening (by zeolite structure standards), which permits a wide range of chemical species to enter, is a principle reason why faujasite catalysts have found wide application in hydrocarbon conversion processes. Zeolite Y preparations were first described in a patent by Breck (1964b) and later by Pitman and Reid (1969). The preparation usually begins with the synthesized sodium form of zeolite Y, NaY. From there it may be ammonium exchanged to yield the NH_4Y type, and then exchanged with metal salts as desired. This route is only one of several that may be used. Assuming now that the desired metal is nickel and its exchange has been made, upon calcination and reduction, a dual functional catalyst should result. According to Hall (1967), acid sites could be formed upon reduction of the transition metal cation by hydrogen at elevated temperatures as the scheme below illustrates.



This reduction of transition metal cations is a major factor in the production of Brönsted acid sites. Benesi (1967) studied reactions of toluene, n-butane, and n-pentane with both hydrogen (Brönsted acid) and hydrogen free (Lewis acid) forms of ammonium zeolites and concluded that Brönsted acids were the seat of activity for toluene disproportionation. As these Brönsted acid sites are generally accepted as responsible for

the cracking activity, i.e. the formation of carbonium ions discussed in the next section, infrared techniques have been developed to study them as discussed by Gates et al. (1979). Transition metals can also be reduced by hydrocarbon reactants. This was demonstrated by Tsutsumi et al. (1972) as an increase in conversion of cumene with pulse number, i.e. with successive slugs of cumene passed over the catalyst sample in helium carrier gas on Ni Y zeolite. Minachev et al. (1974) have investigated the valence states of the metal in a number of transition metal zeolites subjected to various treatments using the techniques of X-ray photoelectronic spectroscopy. They found that Fe, Co, Ni, Pd, Pt, Cu, Ag, and Zn all reduced to metal in hydrogen at temperatures from 422 to 823°K. The tendency was also found for reduction of the Group VIII metals which decrease in reducibility according to : Ni > Co > Fe and Pd > Pt. It was also observed that some of the metals showed a tendency to migrate to the external crystallite surface in a reducing atmosphere. They were ranked according to ease of migration as follows: Ag > Pd > Zn > Cu > Ni > Pt.

Richardson (1971) found no evidence for synergistic effects between metal and acid sites with nickel on various Y zeolite supports. He also observed through benzene hydrogenation and ethane/n-hexane hydrogenolysis that there were two types of sites on nickel. Site I (35%) promoted hydrogenolysis and site II (65% weaker than I) promoted hydrogenation/dehydrogenation. He found the reducibility of 3% nickel faujasite to decrease in order of supports as: NaY > CaY > MgY > NH_4Y. However, synergistic effects between metal and acid sites were found by Ward (1975). It was observed in a series of varying levels of Ni exchange with hydrogen Y zeolite that Brönsted acidity remained constant

with degree of exchange at the same level as the parent hydrogen Y zeolite until a breakpoint where acidity dropped rapidly. This occured at about the 90% exchange level without explanation. Also of interest was the variation of catalyst activity with extent of exchange. The activity reached a plateau at about 40% exchange level and remained constant to the 90% level. Above 90%, activity did not decrease as expected from Brönsted acidity measurements, but increased dramatically. The only explanation offered was the possibility that interaction between the nickel ions and the pi electrons of the aromatic nucleus might be operative.

Therefore there is disagreement in the literature on the related roles of active sites but it appears at this point that if poisoning by sulfur is neglected, nickel on a Y faujasite would be an ideal catalyst for coal derived liquid hydrocracking. With ion exchange properties of zeolites, ease of reduction, and metal loading procedures taken advantage of, a highly active and selective catalyst could be made. In practice, for example, starting with an NH_4Y zeolite, the metal nickel may be cation exchanged in an aqueous solution of nickel nitrate wherein the metal to be deposited forms a cation. These nickel cations must be reduced to nickel metal which can be done by heating in hydrogen, a process which ruptures the bonds between the metal and the zeolite framework which were initially responsible for the high degree of metal dispersion. In this step, there are two related points to consider. First, the location of the cation sites, and second, the diffusion and natural tendency for the free metal to agglomerate into crystallites.

Gallei et al. (1974) discuss in their study of ion exchange in NaX and NaY the six possible groups of cation sites in X and Y zeolites:

I: in the hexagonal prisms,

I′: in sodalite cages adjacent to the six rings of hexagonal prisms,

II: in windows between sodalite and supercages,

II′: projects into the sodalite cages from six rings of site II,

II′′: in the supercages and adjacent to six rings, and

III: elsewhere in the supercages.

The distribution of the cations among the various sites was doubtful at that time. However, the actual position of the cations may not be as important as the effects of metal migration and agglomeration since high dispersion within the matrix affords not only high activity and possible selectivity but also poison resistance.

Lawson and Rase (1970) concluded that to keep nickel crystallites small and well dispersed in the crystal lattice, reduction should be made at a low temperature (589°K) and for long times (7.2×10^4 s). This observation was made using an electron microscope and X-ray diffraction techniques. A more recent investigation by Penchev et al. (1973) studied the temperature dependence of the formation of nickel crystals on types A, X, and Y zeolites with 7 to 8 weight percent nickel. The surface and size of the nickel particles after reduction were determined by gas chromatograph impulse titration in a flow system wherein chemisorption of oxygen in helium flow was used for the nickel samples. Data from the analyses were confirmed by electron microscope. They found, as shown in Figure 2.7, that the maximum surface of nickel in the Y zeolite occured at about 730°K and that above that point sintering of the particles occured with a decrease in the specific

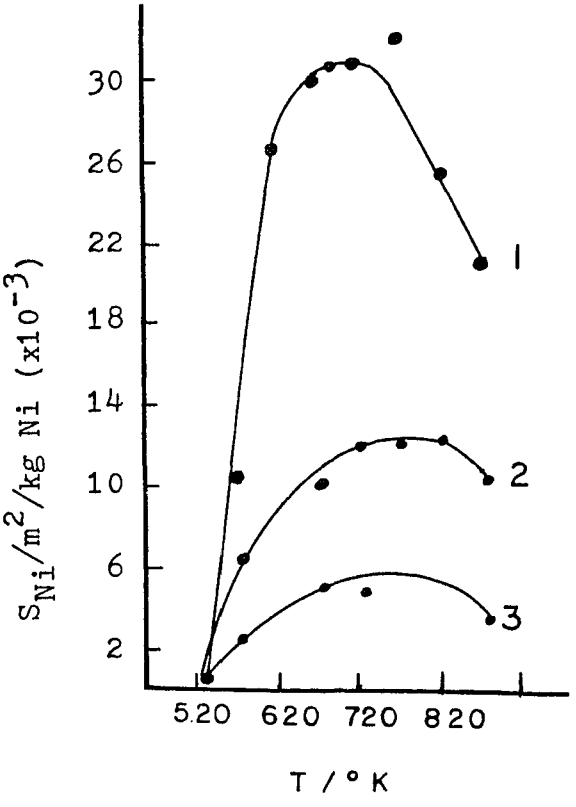


FIGURE 2.7 Dependence of Nickel Surface in the Zeolite on Reduction Temperature: 1, NiA (Ni 7.1 wt%, SiO_2/Al_2O_3 = 2); 2, NiX (Ni 8.1 wt%, SiO_2/Al_2O_3 = 2.6); 3, NiY (Ni 8.0 wt%, SiO_2/Al_2O_3 = 3.8). (Penchev et al., 1973).

surface area. Since it is expected that samples with greater metal surface should have higher activity, reduction temperatures above 730°K should be avoided.

iii) Zeolite Surface Chemistry and Carbonium Ions

Hydrocracking of a hydrocarbon is the cleavage of a C-C bond accompanied by hydrogenation to form two molecules from one. The mechanism involves adsorption of the hydrocarbon on a group of sites with dissociation of a hydrogen atom from the hydrocarbon. Group VIII metals have been found most active in hydrogenation while Brönsted acid sites are thought to be responsible for the carbonium ion formation and its resulting reactions. In the first transition series, maximum activity has been shown for the third subgroup element, nickel. These generalizations are developed in more detail by Sinfelt (1973) and by Dowden (1978).

The concept of sites, introduced by Taylor (1948), states that reaction takes place only on specific locations of the catalyst. A group of these sites may be termed an active center of the catalyst.

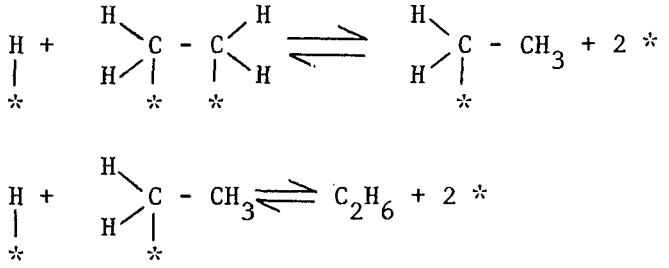
Hydrogenation/dehydrogentation of hydrocarbons on metals is exemplified in early work by Turkevich et al. (1950) with the reaction:

$$C_2H_4 + H_2 \rightleftarrows C_2H_6$$

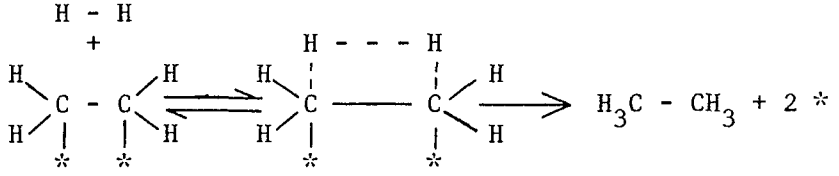
where they observed extensive H-D exchange between the hydrogens of C_2H_4 and D_2. They proposed the following mechanism where * represents surface sites (metals).

$$H_2 + 2\,* \rightleftarrows 2\,H\text{-}*$$

$$2\,* + H_2C\text{-}CH_2 \rightleftarrows H_2C(*)\text{-}CH_2(*)$$



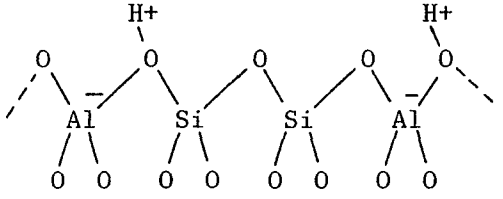
It is also possible that a nondissociated hydrogen molecule reacts with adsorbed hydrogen by the Eley-Rideal mechanism (1941) as shown below for ethylene hydrogenation.



(Gates et al., 1979)

With hydrogenation/dehydrogenation function available from the metal sites, it is also necessary to crack the C-C bonds in order to reduce the structures of coal derived liquid compounds to more usable fuel fractions such as benzene, toluene, xylenes, (BTX).

As was shown earlier, upon reduction, the surface of the zeolite structure may be schematically represented as:



These OH groups are sites that represent potential Brönsted acid sites and are responsible for the formation of carbonium ions. The heteropolar rupture of the C-H bond of a hydrocarbon leads to the formation of either a carbonium ion or a carbanion (Gates et al., 1979):

$$-\overset{|}{\underset{|}{C}} - H \rightarrow -\overset{|}{\underset{|}{C}}^{+} + H^{-}$$

$$-\overset{|}{\underset{|}{C}} - H \rightarrow -\overset{|}{\underset{|}{C}}^{-} + H^{+}$$

The stability of carbonium ion decreases in the order of increasing ionization energies and the electron affinities of the hydrogen and alkyl groups along with the dissociation energy of the C-H bond. The energy required for formation increases with an increase in the number of H atoms attached to the carbon atom from which the hydride ion is abstracted. In order of stability, tertiary > secondary > primary > methyl. This pattern is valid for both ions in solutions and on surfaces.

One of the simplest ways to form a carbonium ion is via abstraction by a hydrocarbon of a proton from a Brönsted acid:

$$H_2C = CHR + H^{+} \rightarrow CH_3CH^{+}R$$

This can then undergo a variety of reactions including double bond shift, isomerization, cracking, and hydrogen exchange (Satterfield, 1980). For example, beta scission, i.e., heterocyclic splitting of C-C bonds with generation of shorter chain olefin molecules:

$$RCH^{+}CH_3 \rightarrow CH_3CH_2 = CH_2 + C^{+}H_2CH_2CH_2CH_3$$

where R = $CH_3CH_2CH_2CH_2CH_2$-, which may rearrange to a more stable structure and finally undergo hydrogen ion transfer. The mechanism of beta scission, and the steps that follow it are generally accepted in the literature as the role of the carbonium ion in cracking reactions (Thomas, 1949, Gary and Handwerk, 1975, and Gates et al., 1979). This concept may be extended to polynuclear aromatic hydrocracking if first a cyclic olefin is formed, then converted to a carbonium ion which is isomerized or cracked. Egan et al. (1962) found that in hydrocracking C_9 to C_{12} alkylcyclohexanes that the C-C bonds in the ring cracked as

readily as those in the side chains. This concept of carbonium ion reactions as applied to catalytic cracking was developed by many investigators and has been reviewed by Oblad et al. (1951), Emmett (1965), and Gates et al. (1979).

iv) Diffusion Limitations

Seven steps are involved in a catalytic process: (Froment and Bischoff, 1979)

a. Transport of reactants from main stream to catalyst pellet surface.

b. Transport of reactants into the catalyst pores.

c. Adsorption of reactants on the sites.

d. Surface chemical reaction.

e. Desorption of products.

f. Transport of products out of the pores to the surface.

g. Transport of products from the surface back to the main fluid stream.

When molecules are nearly the size of the passageway, the rate of diffusion becomes slow and is known as restricted or "configurational" diffusion (Weisz, 1973). This mode is in contrast to both ordinary or bulk diffusion where the mean free path is small relative to the pore diameter and Knudsen diffusion where molecular mean free path greatly exceeds the pore dimension. Zeolitic diffusion is more complex than either bulk or Knudsen diffusion. In the "configurational" mode, molecule-pore wall interations are strong and the rate is influenced by other factors such as the nature and concentration of other adsorbed molecules and the size and location of sites in the zeolite structure.

Also, the extent to which the diffusing molecule interacts with the strong electrostatic fields associated with the cations is another important factor. Whereas order of magnitude estimates may be made for intraparticle diffusivities in the ordinary or Knudsen regimes as shown by Satterfield (1970), the only methods by which configurational diffusivities can be obtained is by experiment. These methods have been employed by Haynes (1975) in great detail and comparison of the results of other investigators has been summarized by Satterfield (1980).

The question of the significance of intracrystalline diffusion when coal derived liquids are processed over large pore zeolites is still unanswered. While it is widely accepted that high molecular weight feeds react within the crystallite, it has been proposed by Thomas and Barmby (1968) that the primary reactions take place on the external surface and that smaller molecules then enter the crystallite matrix. Beecher, Voorhies, and Eberly (1968) studied hydrocracking of mixtures of n-decane and decalin with mordenite catalysts impregnated with palladium and found that acid leaching of the mordenite produces an Al deficient structure of significantly higher catalytic activity. Part of this improvement was credited to a decrease in diffusion resistance. The strong adsorption of high molecular weight hydrocarbons on NaY zeolites was observed by Haynes (1979) with decalin, where a typical Arrhenius plot of overall rate constant gave an activation energy of about 5.5×10^4 kcal/kg mole. He further states that this high activation energy indicates that the reaction was kinetically controlled and there were no significant mass transfer limitations of decalin on NaY zeolite likely.

Therefore, whereas "configurational" diffusion may be rate limiting, it is also responsible for high catalyst activity due to the strong interactions between the molecules and nearby sites.

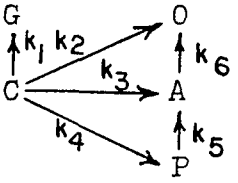
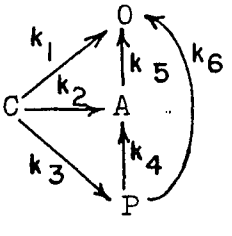
4) Model Compound Studies and Reactions

i) Related Studies

Coal liquefaction mechanisms investigated from 1951 to 1979 were summarized by Mohan and Silla (1981) as shown in Table 2.6. In each case, the products involve mixtures of polynuclear aromatic hydrocarbons. In order to gain further understanding of the mechanisms in both liquefaction and refining of coal derived liquids, many studies have been made using simplified model compounds of these complex mixtures. The hydrocracking of model polynuclear aromatic hydrocarbons has been reported to proceed through a multistep mechanism involving hydrogenation, isomerization, cracking, and rehydrogenation, in that order (Qader and Hill, 1972, Qader, 1973, Brown and Howard, 1975). The primary reactions observed during the hydrocracking of tetralin, anthracene, phenanthrene, and pyrene over nickel surface on silica-alumina were found to be hydrogenation, alkylation, cracking, and pairing, i.e. a cracking reaction where the cyclic structure is preserved and the primary product is isobutane (Flinn et al., 1960, Sullivan et al., 1961, 1964, Langlois and Sullivan, 1970).

The first reaction in the hydrocracking of anthracene as found by Qader and Hill (1972) and by Qader (1973) was the stepwise hydrogenation to di-, tetra-, and octahydroanthracene as shown in Figure 2.8. The cyclohexane rings of the tetra- and octahydroanthracene forms were then isomerized to five membered rings which subsequently cracked to

TABLE 2.6 Coal Liquefaction Mechanism Summary. a) G, Gases; O, Oils; A, Asphaltenes; P, Preasphaltenes (Mohan and Silla, 1981).

kinetic scheme[a]	coal	hydrogen donor solvent	added catalyst	rate constant at 673.15°K, $s^{-1} \times 10^5$
$C \xrightarrow{k1} A+O$	Wyoming	none	none	$k_1 = 5.0$
$C \xrightarrow{k_1} A+O$	Utah	tetralin	none	$k_1 = 62.0$
$C_1 \xrightarrow{k_1} A+O$, $C_2 \xrightarrow{k_2} A+O$	Spitsbergen	none	Ca-Cu-Cr	$k_1 = 11.3$
SAME AS SPITSBERGEN	Pittsburgh	tetralin	none	$k_1 = 5033.3$
SAME AS SPITSBERGEN	Pittsburgh extract	none	$ZnO/ZnCl_2$	$k_1 = 400.0$ $k_2 = 10.3$
$C \xrightarrow{k_1} A \xrightarrow{k_2} O$	Pittsburgh Anthraxylon	none	SnS,NH_4Cl	$k_1 = 45.0$ $k_2 = 1.8$
$C \xrightarrow{k_1} A$, $C \xrightarrow{k_2} O$	bituminous	tetralin	none	$k_1+k_2 = 6.5$
$C \xrightarrow{k_1} A \xrightarrow{k_2} O$, $C \xrightarrow{k_3} O$	Japan	decrystallized anthracene oil	red-mud and sulfur	$k_1 = 6.2$ $k_2 = 8.2$ $k_3 = 28.3$
	Belle Ayr	hydrogenated phenanthrene	none	$k_1 = 248.7$ $k_4 = 329.8$ $k_2 = 142.5$ $k_5 = 40.0$ $k_3 = 257.7$ $k_6 = 122.5$
	Kentucky	tetralin	none	$k_1 = 0.7$ $k_4 = 0.1$ $k_2 = 1.25$ $k_5 = 0.1$ $k_3 = 2.0$ $k_6 = 0.1$

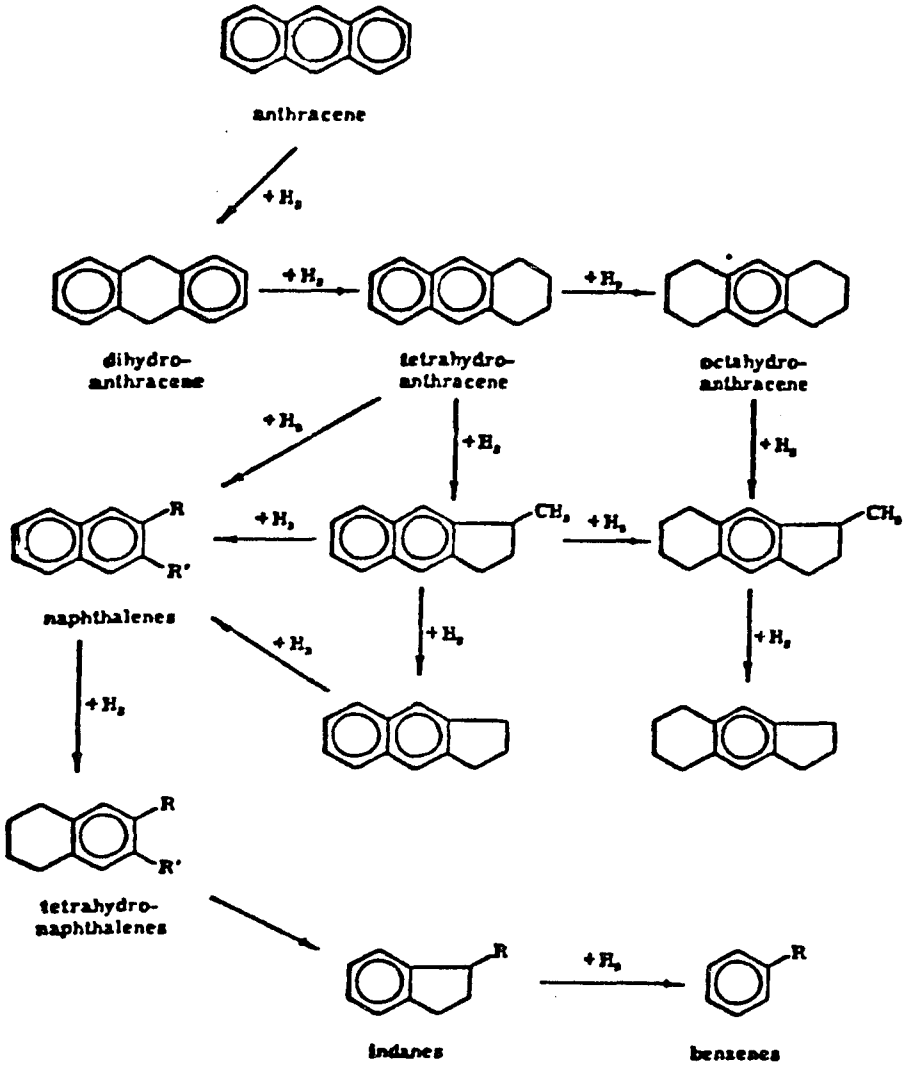


FIGURE 2.8 Mechanism of Anthracene Hydrocracking (Qader and Hill, 1972, Qader, 1973)

naphthalenes. The latter are then converted to benzene via hydrogenation, isomerization, and cracking of one of the rings.

Sullivan et al. (1961, 1964) and Langlois and Sullivan (1970) found three types of reactions occuring in hydrocracking phenanthrene:

a. Saturation and cleavage of one of the terminal rings to form a paraffin and bicyclic such as tetralin.

b. Ring saturation and cleavage of the central ring to form methylcyclohexane and ethylcyclohexane.

c. The predominant reaction was composed of a complex sequence of hydrogenation, cracking, and alkyl transfer.

The type b. reaction found by Sullivan is important with respect to work by Wu and Haynes (1975) where central ring cracking of phenanthrene was indicated on a Cr_2O_3-Al_2O_3 catalyst by the presence of significant amounts of biphenyl and 2-ethyl biphenyl in the products.

The hydrogenation of linear multi-ring aromatic compounds of three rings or more was found by Clar (1964) to be initiated by the addition of hydrogen to a ring position other than the end ring.

Highly condensed polynuclear aromatics tend to be refractory and difficult to study for catalytic reactions. Therefore, for convenience, most of the previous studies were carried out in batch autoclaves. This procedure has its advantages, but can mask specific catalytic activities by catalyst deactivation and product inhibition. Also prone to mask catalytic effects is free radical chemistry and thermal cracking. Vernon (1980) studied the free radical chemistry and the role of molecular hydrogen on model coal compounds and found that molecular hydrogen can participate directly in free radical reactions under coal liquefaction conditions. Dibenzyl-tetralin-hydrogen reactions were

studied and cracking occured on the central bond as shown in Figure 2.9. In the study of catalytic hydrocracking of model compounds, this region of pyrolysis (672 to 773°K) should be avoided to prevent thermal cracking from masking catalytic effects. However, the work is of interest as it was noted that the use of an effective donor solvent with molecular hydrogen should produce high liquid yields at lower hydrogen pressures and with lower hydrogen consumption. An extension of this into the catalytic hydrocracking region would be of primary economic importance to a commercial process. There may be limitations imposed however, as it was found by Cronauer et al. (1979) that the reaction of dibenzyl to break the C-C bond occured purely thermally and was independent of the nature of the hydrogen donor solvent present.

ii) Decalin as Hydrogen Donor Solvent

From the previous discussion, it is not clear as to the role of a donor solvent in thermal cracking where free radical mechanisms predominate. The important point is to avoid the thermal region so that catalytic interactions with the donor may be observed. Moore (1967) noted little or no reaction for decalin, methylcyclopentane, toluene, and similar compounds below 773°K. He also noted that decalin dehydrogenated to give naphthalene. Clarification of the role of a donor solvent was made by Ratto et al. (1980). In their study of fully deuterated tetralin, deuterium gas and bituminous coal, four main reactions were found to take place:

a. Direct transfer of hydrogen to coal; the donation or addition mechanism.

b. Direct hydrogenation of coal from the gas phase deuterium.

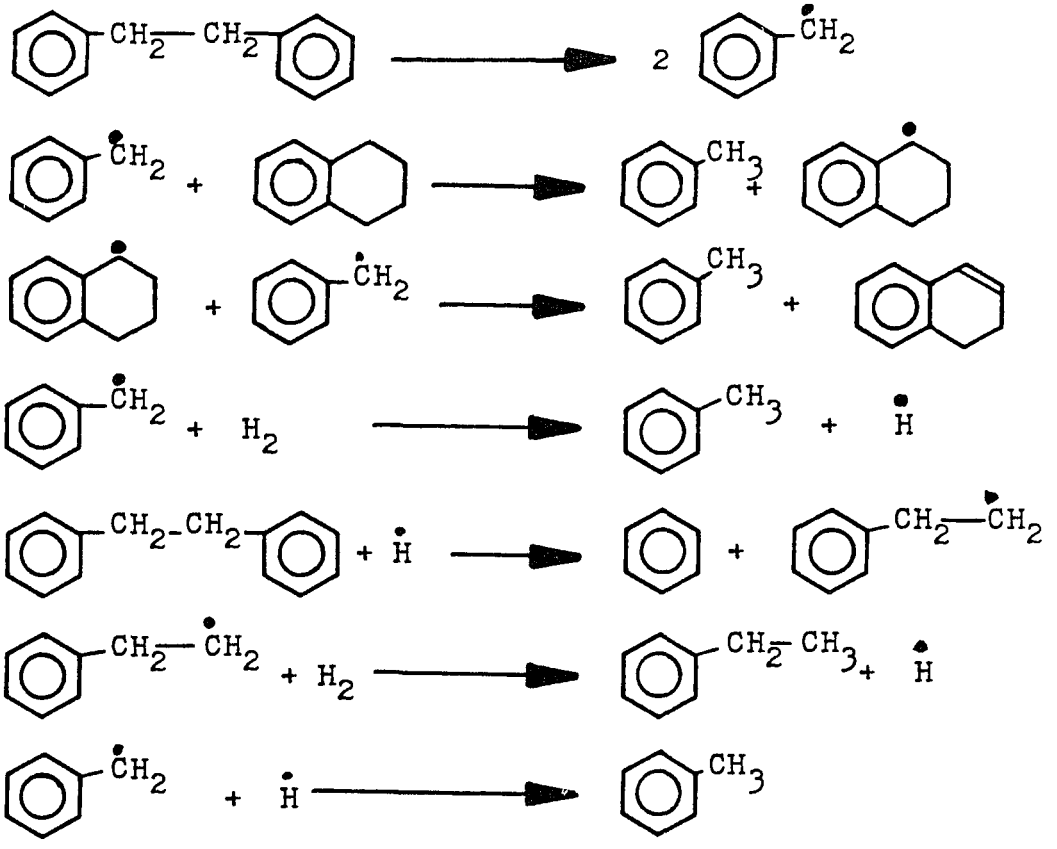


FIGURE 2.9 Reaction Scheme for the Pyrolysis of Dibenzyl in the Presence of Tetralin and Molecular Hydrogen (Vernon, 1980)

c. Indirect hydrogenation of coal by the gas phase via tetralin.

d. Tetralin-d_{12} in isotopic exchange of its deuterium with hydrogen in the coal. This work was performed thermally with the reaction pathways for tetralin developed as shown in Figure 2.10.

It appears then that if the decalin to naphthalene reaction is successful by catalytic routes, a large amount of hydrogen could be made available for reaction with the aromatics of coal derived liquids. Patzer et al. (1979) used tetralin as a donor solvent initially in a catalytic reaction and found that the reverse reaction may occur, consuming hydrogen and forming decalin. Therefore, dehydrogenation of either decalin or tetralin is essential to initiate a donor mechanism.

Many investigations have been made in the reactions of decalin. For this study, its dehydrogenation and related reactions are presented. Early work by Bloch and Thomas (1944) with decalin over silica-alumina-zirconia catalysts at 672 to 773°K showed that direct scission of decalin formed C_4 and C_6 cyclic fragments. It was postulated that these fragments may form olefins or receive hydrogen from decalin to give saturated products. They also found that the alkyl benzenes formed were similar to those formed from tetralin and that the naphthalene formed was through the tetralin intermediate rather than direct from decalin. Thermal reactions may have been present as the temperatures were in that region.

Hydrogen transfer over silica-alumina was investigated by Blue and Engle (1951) wherein cis-decalin and tetralin were found to be hydrogen donors and trans-decalin acted as a diluent since it was unreactive at the conditions studied. 1-butene and isobutene were used as hydrogen

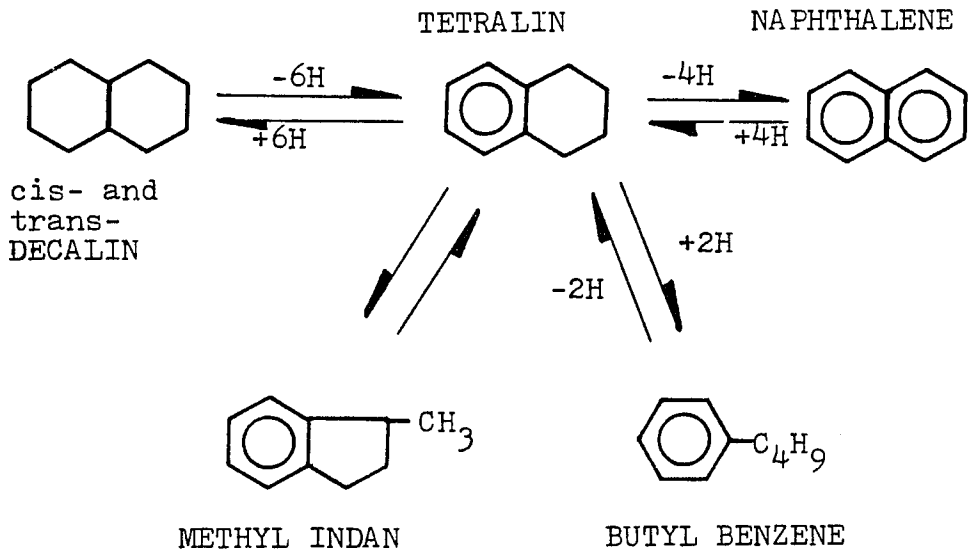
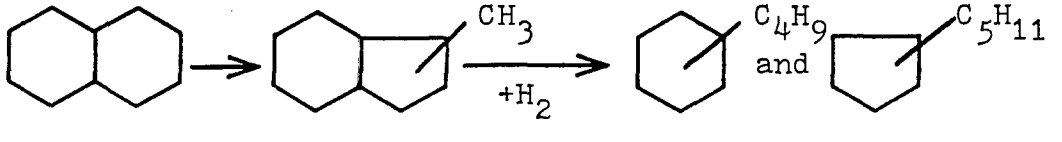


FIGURE 2.10 Reaction Pathways of Tetralin During Liquefaction (Ratto et al., 1980)

acceptors. They concluded that the mechanism of transfer proceeds through an ionic mechanism over the acidic catalyst surface. This conclusion is reinforced if one considers the structures of cis- and trans-decalin. Since cis-decalin has two hydrogens on tertiary carbons on one side of the molecule, it could make two point contact more readily than trans-decalin.

Both thermal and catalytic dehydrogenation of decalin was done by Ritchie and Nixon (1967) on platinum-alumina catalysts at 11.15 to 32.01 bars over a temperature range of 623 to 974°K. They also noted higher dehydrogenation activity of cis-decalin compared to trans-decalin and that as pressure increased, naphthalene yield decreased. Several conclusions are made in their work. First, the second reaction of tetralin to naphthalene was 1 to 1.5 orders of magnitude faster and had an activation energy about three times greater than the first step of decalin to tetralin. They found the trans-isomer of decalin to be reactive, but not to the extent of the cis- isomer. The isomerization of decalin from cis- to trans- was 5 to 10 times faster than the rate for trans- to cis-. For dehydrogenation the rate of cis- was 6 to 30% faster than trans-decalin.

Should hydrocracking of decalin occur instead of dehydrogenation, another reaction path develops. Yamadaya et al. (1977) hydrocracked decalin over supported nickel-tungsten at high pressures (104.4 bars) in a fixed bed continuous flow system, and found that methylperhydroindenes and C_{10}-naphthenes were formed as shown below.



Therefore, to process coal liquids, a combination of reactions is necessary. There must be dehydrogenation of the solvent (decalin) to supply hydrogen and hydrogenation and cracking of the coal liquid. This was demonstrated by Dziewiecki et al. (1979) in a continuous flow reactor with a fixed bed containing supported Ni-Moly catalyst using decalin and a coal extract at 723°K, 277 bars, and a space velocity of 1.39×10^{-4}/s. At this high pressure, they postulated that catalysts active in decalin dehydrogenation should exhibit the same property in the hydrogenation of coal extracts assuming that dehydrogenation/ hydrogenation of decalin is reversible and that: a) the mechanism is the same and b) hydrogen introduced into the system hydrogenates only the naphthenic compounds and not all ring compounds. Since benzene derivatives are more stable, this should not occur.

iii) Fluorene Reactions

It has been shown that much work has been done on the reactions of the donor solvent decalin. However, studies of the hydrocracking of the model coal liquid compound fluorene are very limited in the literature. These are summarized in Table 2.7 for discussion. As reviewed by this author, little if any work has been done using a flow reactor system incorporating a metal loaded zeolite to hydrocrack fluorene as a model compound in a typical donor solvent such as decalin to obtain products similar to motor fuels. However, much insight may be drawn from the previous fluorene work in other reaction systems.

Oltay et al. (1973) found that at 672 to 756°K in hydrogen pressures up to 380 bars the reaction sequence shown in Figure 2.11 occurs. The yield of route I was 90% and by route II and III about 8

TABLE 2.7 Previous Fluorene Hydrocracking Studies

Investigator	Reactor	Catalyst or Mode	Solvent
Oltay et al. (1973)	Batch	Thermal	None
Nakatsuji et al. (1978)	Batch	$ZnCl_2/CuCl_2$	None
Salim (1981)	Batch	$ZnCl_2/AlCl_3$	cyclohexane
Graber and Huttinger (1982)	Flow	Thermal	None

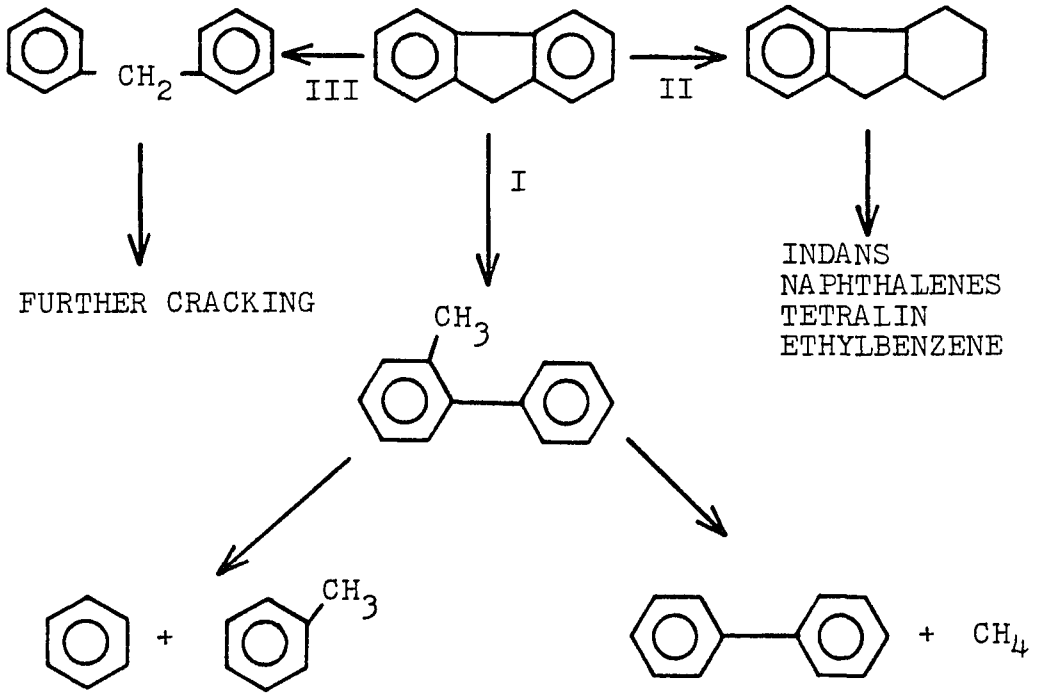
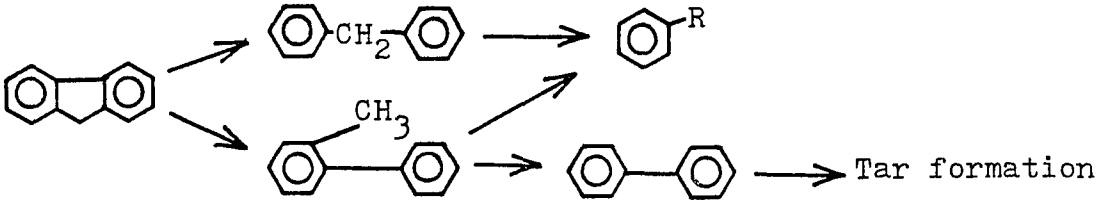


FIGURE 2.11 Reaction Sequence in the Thermal Hydrocracking of Fluorene (Oltay et al., 1973)

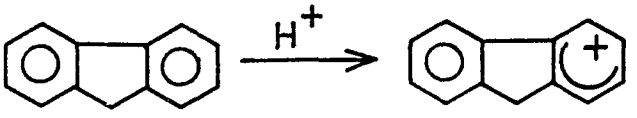
and 0.5 mol % respectively. In their study, a major portion of fluorene remained liquid due to the high hydrogen pressure so that sufficient hydrogen transfer to the liquid phase was a prerequisite for hydrocracking. They also proposed the scheme shown in Figure 2.12 for the formation of cracked products by route II.

A more general study by Nakatsuji et al. (1978) was the hydrocracking of many derivatives of polynuclear aromatics, of which fluorene was one. After reaction at 672°K for 1.08 x 10^4 s in a batch autoclave with Zn $Cl_2/CuCl_2$ molten salt catalyst, the weight % of products were found as listed in Table 2.8. Including the gases which may also be burned as fuel, 66.3 wt. % of the products (group 1-4) may result in usable fuels.

In a more detailed study by Salim (1980) using $ZnCl_2$ ($AlCl_3$ was not reactive) at 598°K and 111.3 bars in a batch autoclave, fluorene was hydrocracked with high liquid yields and tar being the products. Networks were explained in terms of the carbonium ion mechanism with the following reaction sequences presented: cracking of the central ring at either the phenyl-phenyl bond or phenyl-methyl bond with 97% conversion of fluorene observed.



In terms of the carbonium ion mechanism proposed:



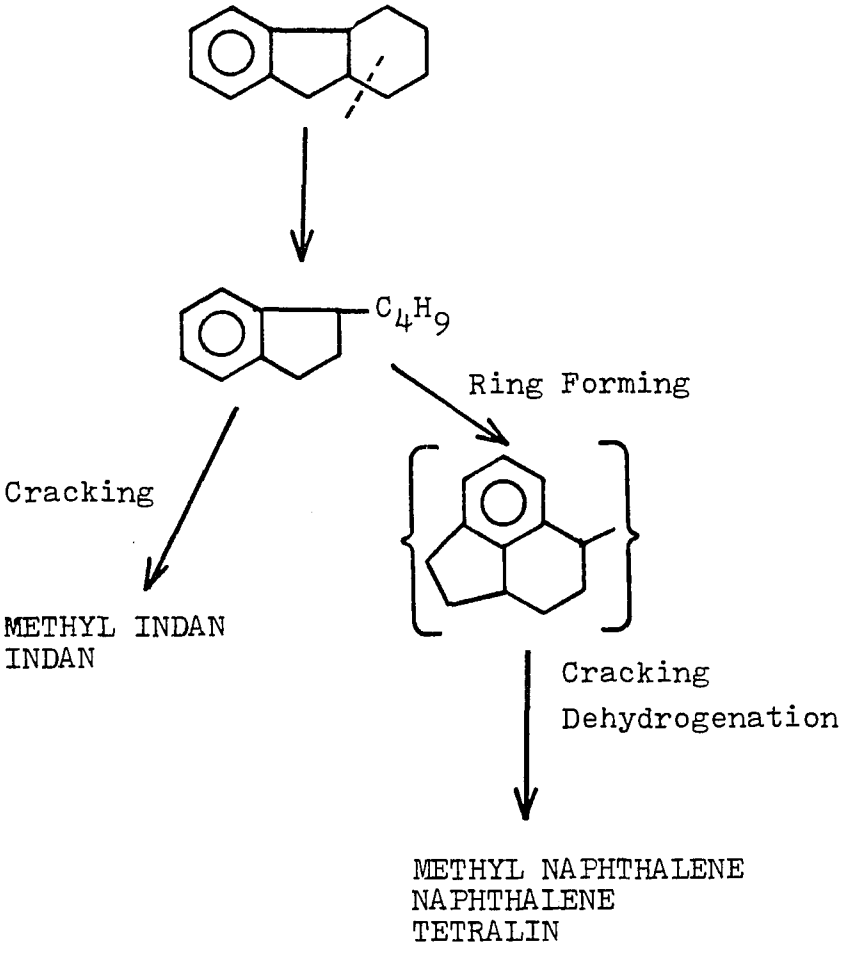
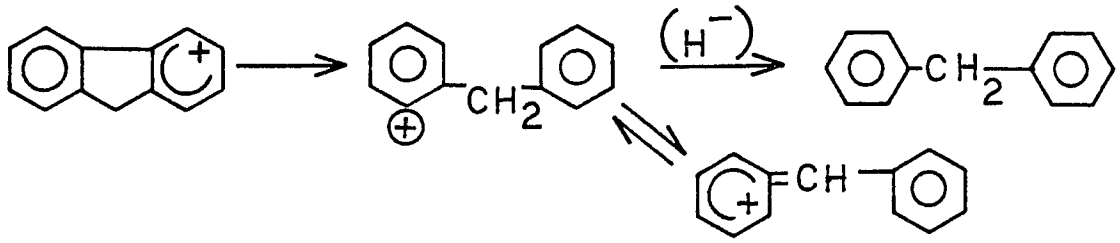


FIGURE 2.12 Formation of Cracking Products From Route II (Oltay et al. 1973)

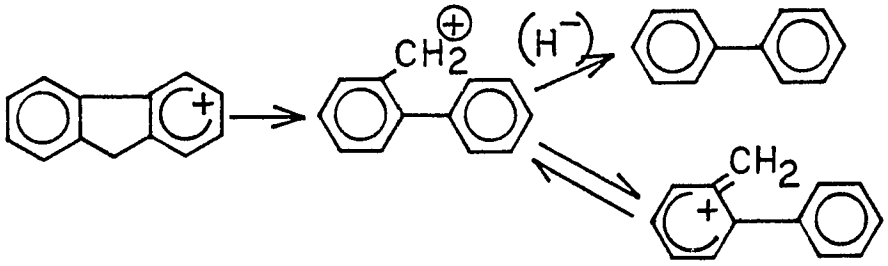
TABLE 2.8 Products of Fluorene Hydrocracking (Nakatsuji et al., 1978)

	Compound Group	Weight %
1.	C_1 to C_4 gases	30.6
2.	C_5 to C_7 alkanes	4.2
3.	cycloalkanes	6.5
4.	monocyclic aromatics	25.0
5.	indans, tetralins, bicyclics (biphenyls)	14.4 (10.5)
6.	tricyclic aromatics	17.5
7.	coke	1.9

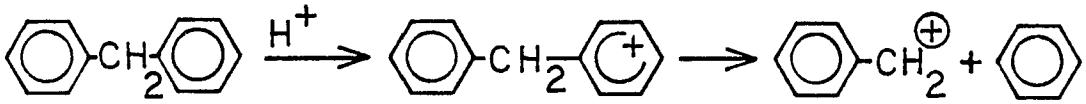
which can now add another ring or undergo cleavage of the central ring. Cracking can also occur at the phenyl-phenyl bond with the resulting carbonium ion stabilized:



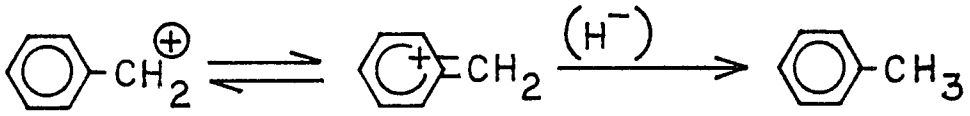
Cracking at the phenyl-methyl bond was proposed to result in formation of a primary carbonium ion which is also resonance stabilized:



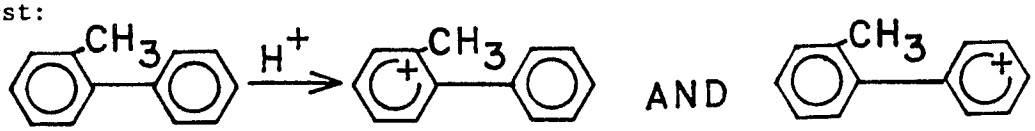
Then, for cracking of diphenylmethane:



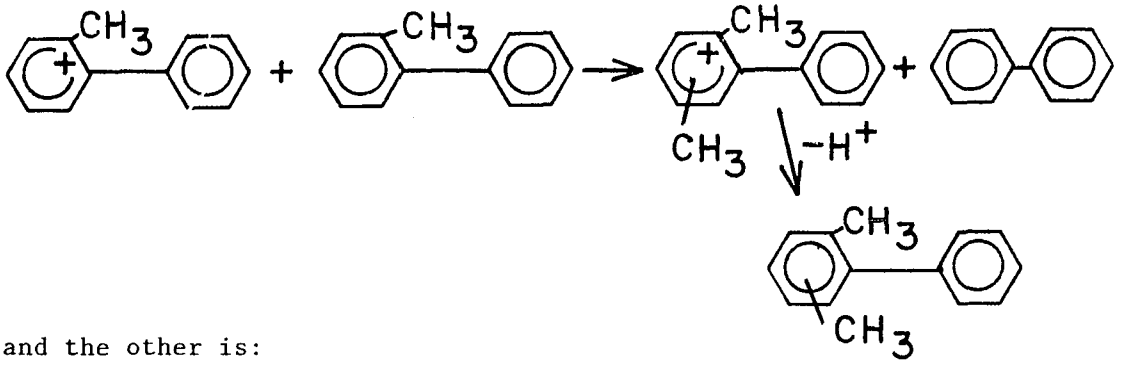
and:



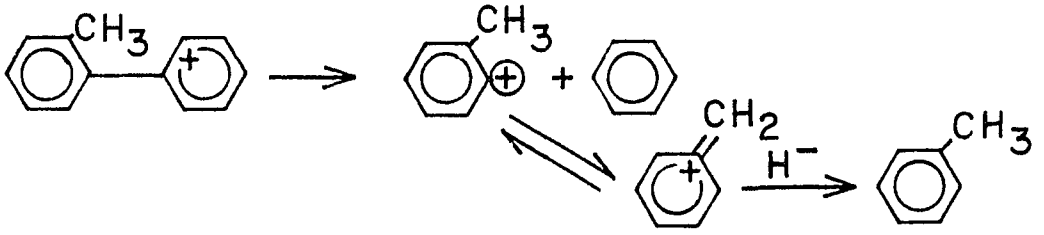
Finally, for the cracking and disproportionation of methyl biphenyl, first:



wherein one route is:



and the other is:



These schemes were proposed by the author based on the theory of carbonium ion formation and reactions and the products observed from the experimental work.

Finally, thermal hydrogasification of fluorene by Gräber and Huttinger (1982) showed that the reaction behavior of the methylene bridge in fluorene was very stable compared with that in diphenyl methane. This reaction by a free radical mechanism (867 to 1273°K) is shown in Figure 2.13. In this scheme, undesirable heavier compounds may be formed. It would also appear from the reaction paths that a catalytic donor process would produce benzenes without the undesirable heavier compounds being formed by free radicals.

iv) Coking Problems

In hydrocracking fluorene and higher aromatics, a signficiant portion of the feedstock may be converted to a carbonaceous (coke) deposit on the catalyst. This leads to deactivation of the catalytic

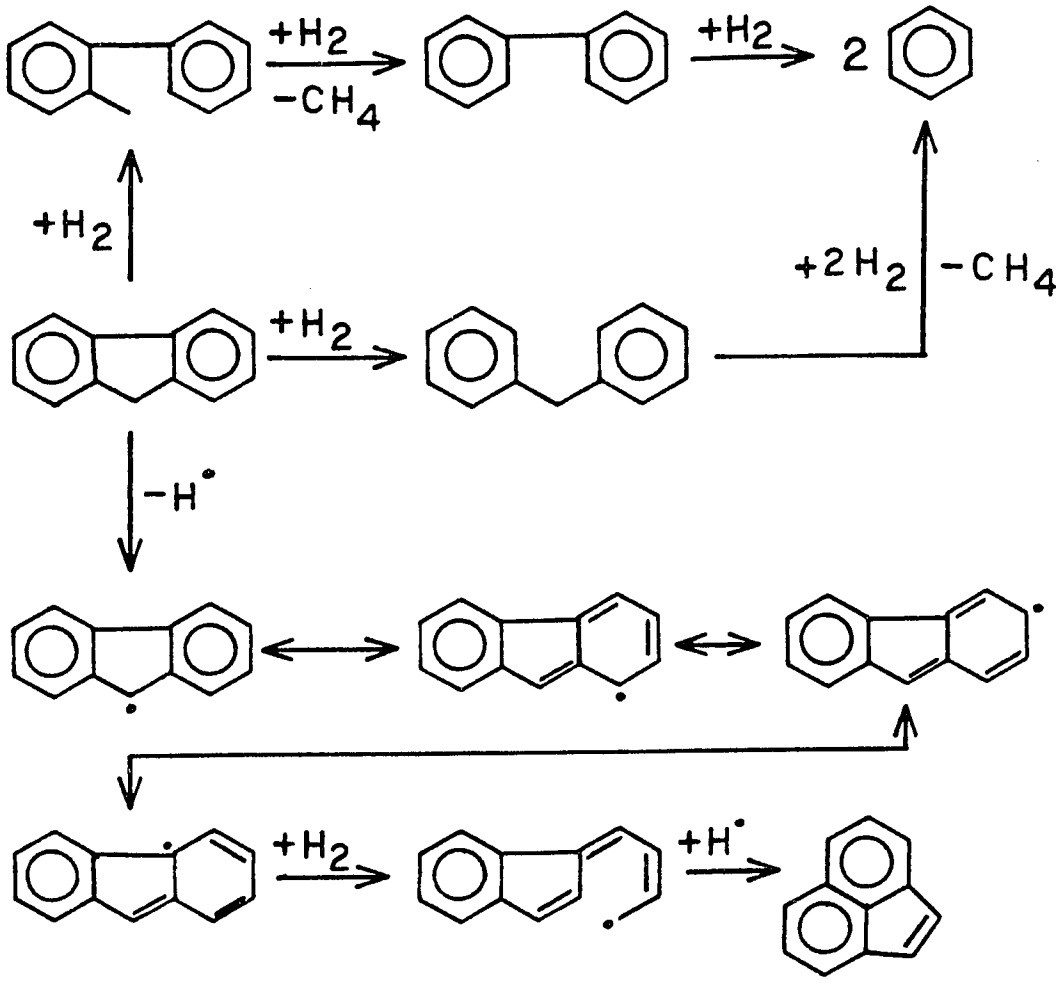


FIGURE 2.13 Primary Reactions in Hydrogasification of Fluorene (Gräber and Huttinger, 1982)

sites, loss of selectivity, and requires either hydrogen recycle or regeneration (burning off of the coke in air) to keep coke levels low on the surface (Otani, 1970). Appleby et al. (1962) fed a variety of heavy polynuclear aromatics including fluorene to a fixed bed reactor containing fresh silica-alumina catalyst to form coke and by regeneration of the catalyst found that fluorene yielded 8.7 wt. % of catalyst weight as coke. Compared to benzene (0.06 wt. % coke) the amount from fluorene is signficiant. This was performed at atmospheric pressure for 900 s at 773°K. However, Rohrer and Sinfelt (1962) explained that hydrogen's role in the system removes these residues, maintaining catalyst activity. This was investigated by passing helium over the catalyst as a carrier instead of hydrogen.

In polynuclear aromatic coking, two approaches can be taken to reduce deactivation. First, a more active catalyst may be used which lowers the temperature enough to minimize free radical reactions. Secondly, the coke precursors can be quenched by hydrogen donors. Assuming that coke will be formed, for a given catalyst, feedstock, and temperature, good correlation between feedstock conversion and coke yield has been observed. This relation may be expressed as the Voorhies (1945) equation or "coke clock":

$$C_c = a\ \tau_c^n$$

where a = feedstock, catalyst, temperature coefficient,

τ = catalyst residence time,

n = constant.

Thus the % carbon is logarithmically proportional to the catalyst exposure time since regeneration. Overall, the rate of coke formation will increase with acid strength of the catalyst, basic strength of the

hydrocarbon reactant, and acid site density. Reflecting this on zeolites used for this study, coking must be accounted for in reaction evaluation.

5) Literature Review Conclusions

i) Model compounds will be required to investigate the kinetics and mechanism involved in hydrocracking the polynuclear aromatics of coal derived liquids.

ii) A dual functional catalyst is required which contains both acidic sites to form carbonium ions that proceed on to cracking, isomerization, etc. and metal sites for hydrogenation/dehydrogenation activity. Large pores as contained in Y faujasites are necessary and the metal nickel is highly active for hydrogenation/dehydrogenation.

iii) Decalin may be used as a donor solvent as it has been shown to proceed through tetralin to naphthalene thereby giving up hydrogen. Its role as a donor solvent must be determined as several routes have been proposed but it is not clear as to which is operative in fluorene reactions. Decalin may also proceed on its own via hydrocracking to other compounds.

iv) Studies of fluorene hydrocracking, especially on metal loaded zeolites in flow systems, are limited and its conversion to fuel fractions should be determined as a model for coal derived liquid refining.

v) Coking and deactivation play an important role in catalyst maintenance and extension of the work in the petroleum processing industry should be employed for coking problems in the decalin/fluorene/hydrogen catalytic system.

vi) Thermal reactions (free radical mechanisms) should be avoided as they tend to mask catalytic effects and increase coke formation.

vii) Finally, a composite reaction scheme, based on the literature reviewed, has been drawn for decalin and fluorene as shown in Figure 2.14 and 2.15 respectively as a starting point to determine reaction pathways. The nature of the interactions between decalin, fluorene, hydrogen and catalysts combined in a flow system to model coal liquid reactions is not clearly understood or defined in the literature.

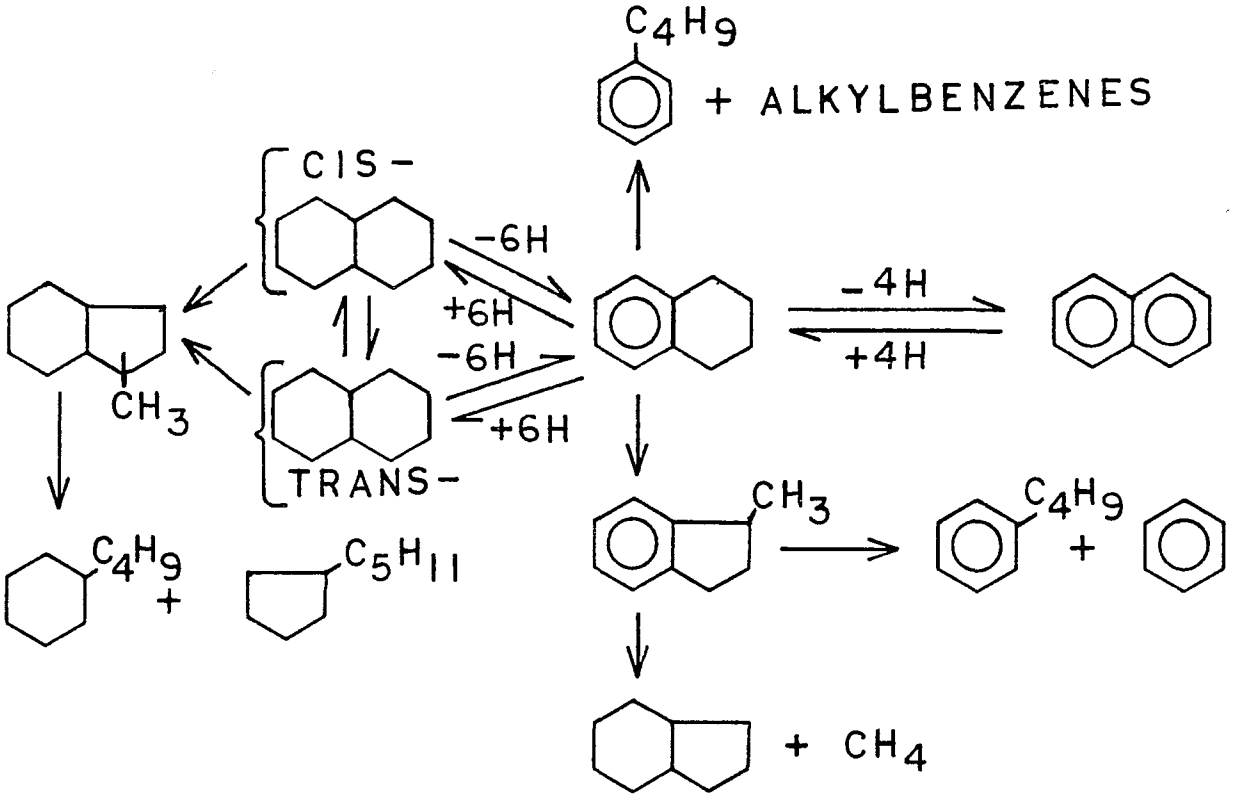


FIGURE 2.14 Decalin Composite Reaction Scheme

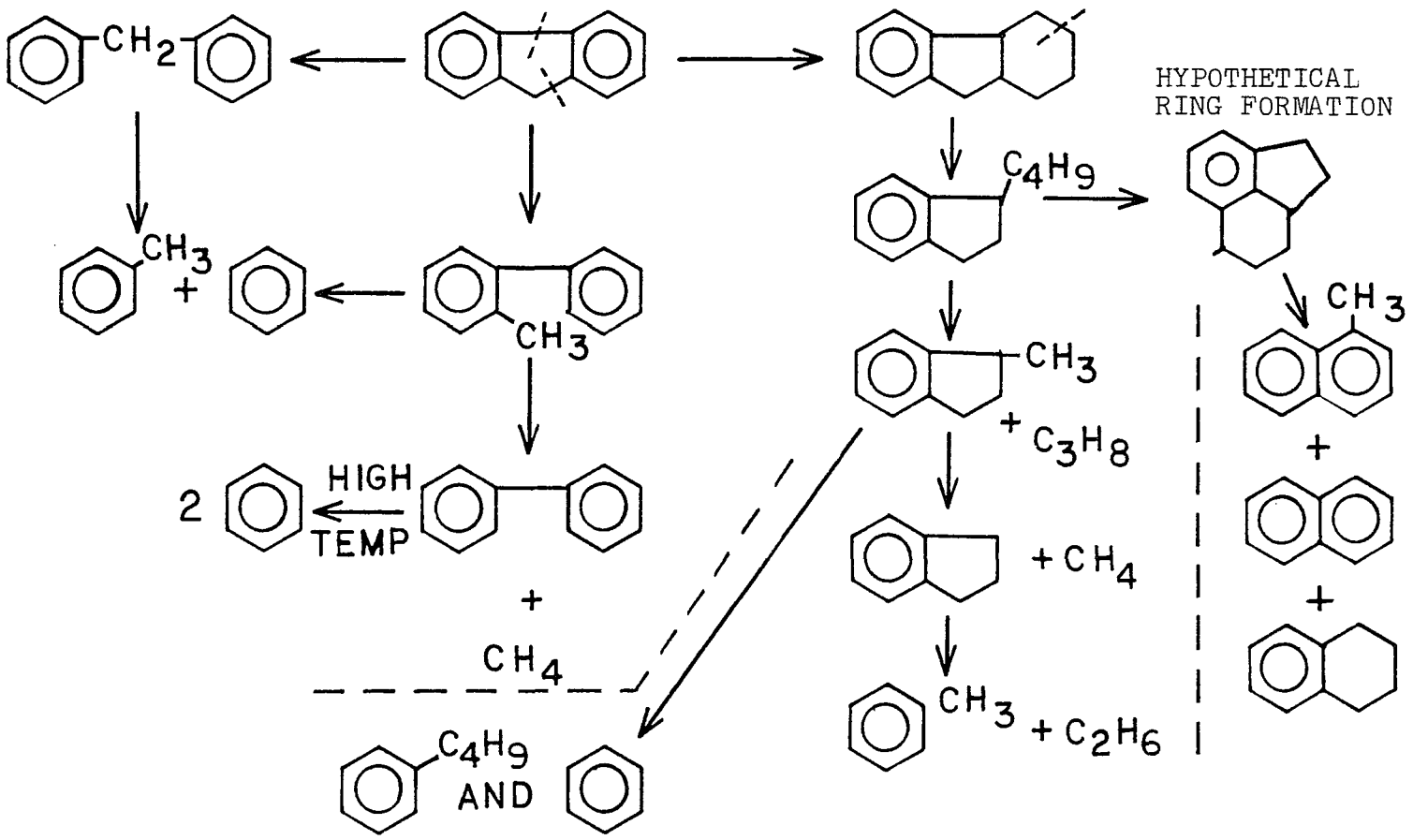


FIGURE 2.15 Fluorene Composite Reaction Scheme

6) Literature Cited

Appleby, W.G., J.W. Gibson, and G.M. Good, Ind. and Eng. Chem. Proc. des. and Develop. 1(2), 102-110 (1962).

Bartle, K.D. and M. Zander, Erdöl and Kohle, 36(1), 15-22 (1983).

Beecher, R., A. Voorhies, Jr., and P. Eberly, Jr., Ind. Eng. Chem. Prod. Res. Develop., 7(3), 203-209 (1968).

Benesi, H.A., J. Catal., 8, 368-374 (1967).

Berg, L., F.P. McCandless, Hemant Bhatia, and Angong Yeh, Energy Progress, 2(4), 236-238 (1982).

Bergins, F. and J. Billwiller, Ger. Patent 301,231 (1913).

Bloch, H.S. and C.L. Thomas, J. Am. Chem. Soc., 66, 1589-1594 (1944).

Blue, R.W. and C.J. Engk, Ind. and Eng. Chem., 43(2), 494-501 (1951).

Breck, D.W., J. Chem. Ed., 41(12), 678 (1964a).

Breck, D.W. U.S. Patent. 3,130,007 (1964b).

Brown, R.R. and J. Howard, Am. Chem. Soc. Div. Pet. Chem. Prepr. 20, 785 (1975).

Brunson, R.J., Fuel, 58, 203-207 (1979).

Chen, N.Y. and P.B. Weisz, Chem. Eng. Prog., Symp. Series 63, 86 (1967).

Clar, E., Polycyclic Hydrocarbons, Academic Press, New York (1964).

Cronauer, D.C., D.M. Jewell, Y.T. Shah, and R.J. Modi, Ind. Eng. Chem. Fundam., 18(2), 153 (1979).

Cummings, A.D., Discovery, 9, 54-57, February (1948).

Cusumano, J.A., R.A. Dalla Betta, R.B. Levy, Catalysis in Coal Conversion, Academic Press, New York (1978).

Dowden, D.A., Catalysis, Vol. 2, The Chem. Soc., London, Ch. 1, p. 1 (1978).

Dziewiecky, Z., M. Ihnatowicz, and A. Makowski, Fuel, 58, 737-740 (1979).

Egan, C.J., G.E. Langlois, and R.J. White, J. Am. Chem. Soc. 84, 1204 (1962).

Eley, D.D. and E.K. Rideal, Proc. R. Soc. London, Ser. A, 178, 429-452 (1941).

Emmett, P.H., Catalysis Then and Now, Franklin, Englewood, N.J. (1965).

Fischer, F. and H. Tropsch, Ger. Patent 484,337 (1925).

Flinn, R.A., O.A. Larson, and H. Beather, Ind. and Eng. Chem., 52, 153 (1960).

Froment, G.F. and K.B. Bischoff, Chemical Reactor Analysis and Design, J. Wiley, New York (1979).

Furlong, L.E., E. Effron, L.W. Vernon, and E.L. Wilson, Chem. Eng. Prog., 72(8), 69, (1976).

Gallagher, J.P., W.H. Humes, and J.O. Siemssen, Chem. Eng. Prog., 75(6), 56-62 (1979).

Gallei, E., D. Eisenbach, and A. Ahmed, J. of Catal., 33, 62-67 (1974).

Gary, J.H. and G.E. Handwerk, Petroleum Refining Technology and Economics, Marcel Dekker, New York (1975).

Gates, B.C., J.R. Katzer, G.C.A. Schuit, Chemistry of Catalytic Processes, McGraw-Hill, New York (1979).

Gräber, W.-D., and K.J. Huttinger, Fuel, 61, 505-509 (1982).

Haggin, J., "Interest in Coal Chemistry Intensifies", Chem. and Eng. News, 17-26, Aug. 9, 1982 (a).

Haggin, J., Chem. and Eng. News, 9-15, Dec. 13, 1982 (b).

Hall, W.K., Chem. Eng. Progr. Symp. Ser. 63, 68 (1967).

Haynes, H.W., Jr., Chem. Eng. Sci., 30, 955-961 (1975).

Haynes, H.W., Jr., "D.O.E. Quart. Report", April 1 - June 30, 1979, FE-2727-7.

Haynes, H.W., Jr., Unpublished Research Proposal, U. Miss. (1977).

Langlois, G.E. and R.F. Sullivan, Am. Chem. Soc. Adv. in Chem. Ser. 77, Ch. 3, R.F. Gould, ed. (1970).

Lawson, J.D. and H.F. Rase, Ind. and Eng. Chem., Prod. Res. Dev., 9(3), 317-324 (1970).

McBain, J.N., The Sorption of Gases by Solids, Rowtledge and Kegan Paul, London (1932).

Miale, J.C., N.Y. Chen, and P.B. Weisz, J. Catal., 6, 278 (1966).

Minachev, Kh.M., G.V. Antoshin, and E.S. Shpiro, Izv. Akud. Nauk SSSR, Ser. Khim. 1012 (1974).

Mohan, G. and H. Silla, Ind. Eng. Chem., Proc. Des. Dev., 20, 349-358 (1981).

Moore, R.N., R.M. Engelbrecht, J.C. Hill, and L.J. Spillane, Am. Chem. Soc. Div. Pet. Chem. Prepr., 12(3), 101-115 (1967).

Nakatsuji, Y., Y. Ikkaku, M. Nomura, and S. Kikkawa, Bull. Chem. Soc. Japan, 51(12) 3631-3634 (1978).

Nowacki, P., Coal Liquefaction Processes, Noyes, Park Ridge, New Jersey, 320-322 (1979).

Oblad, A.G., T.H. Milliken, and G.A. Mills, Adv. Catal., 3, 199 (1951).

Oltay, E., J.M.L. Penninger, and W.A.N. Konter, J. Appl. Chem. Bistechnol., 23, 573-579 (1973).

Otani, S., Chem. Eng., 77(16), 118 (1970).

Owen, J., Fuel, 60, 755-761 (1981).

Patzer, J.F., R.J. Farrauto, and A.A. Montagna, Ind. Eng. Chem. Process Des. Dev., 18(4), 625-630 (1979).

Penchev, U., N. Davidova, V. Kanazirev, H. Mincher, and Y. Neinska, Adv. in Chem. Series 121, 461-468 (1973).

Pitman, J.C. and L.J. Reid, U.S. Patent 3,433,589 (1969).

Qader, S.A. and G.R. Hill, Am. Chem. Soc. Div. Fuel Chem. Prepr., 16, 93 (1972).

Qader, S.A., J. Inst. Pet., 59, 178 (1973).

Ratto, J.J., L.A. Heredy, and R.P. Skowronski, Am. Chem. Soc. Symp. Series 139, 347-369 (1980).

Richardson, J.T., J. of Catal., 21, 122-129 (1971).

Riesz, C.H. and H.S. Weber, J. Am. Oil Chem. Soc. 41, 464 (1964).

Ritchie, A.W. and A.C. Nixon, Am. Chem. Soc. Div. Pet. Chem. Prepr. 12(3), 117-147 (1967).

Rohrer, J.C. and J.H. Sinfelt, J. Phys. Chem. 66(5), 1193-1194 (1962).

Salim, S.S., "Hydrogenation and Cracking of Coal Related Fused Ring Structures using $ZnCl_2$ and $AlCl_3$ Catalyst", Ph.D. Dissertation, U.C. at Berkley (1980), ERA #1832, 6, BL-11512, Jan.-Feb. 1981.

Satterfield, C.N., Mass Transfer in Heterogeneous Catalysis, MIT Press, Cambridge, Mass., (1970).

Satterfield, C.N., Heterogeneous Catalysis in Practice, McGraw-Hill, New York (1980).

Sinfelt, J.H., Adv. Catal., 23, 91 (1973).

Smith, H.A., Catalysis, Vol. V, P.H. Emmett, ed., Reinhold, New York (1957).

Solomon, P.R., A.C.S. Symp. Series 169, A.C.S., Washington, D.C., 61-71, (1981).

Sullivan, R.F., C.J. Egan, G.E. Langlois, and R.P. Seig, J. Am. Chem. Soc., 83, 1156 (1961).

Sullivan, R.F., C.J. Egan, and G.E. Langlois, J. Catal., 3, 183 (1964).

Taylor, H.S., Proc. R. Soc., A108, 105 (1925).

Thomas, C.L., Ind. Eng. Chem., 41, 2564 (1949).

Thomas, C.L. and D.S. Barmby, J. Catal., 12, 341 (1968).

Tsutsumi, K., S. Fuji, and H. Takahashi, J. Catal., 24, 8 (1972).

Turkevich, J., F. Bonner, D.O. Schissler, and A.P. Irsa, Discuss. Faraday Soc., 8, 352 (1950).

Venuto, P.B. and E.T. Habib, Catal. Rev.-Sci. Eng., 18(1), 39 (1978).

Vernon, L.W., Fuel, 59(2), 102-106 (1980).

Vick, G.K. and W.R. Epperly, Science, 217 (4557), 311-316 (1982).

Voorhies, A., Jr., Ind. Eng. Chem., 37(4), 318 (1945).

Ward, J.W., J. of Catal., 38, 351 (1975).

Weast, R.C., ed., Handbook of Chemistry and Physics, 54th ed., CRC Press, Cleveland, Ohio (1973).

Weisz, P.B., Chem. Tech., 3(8), 498 (1973).

Wiser, W.H., S. Singh, S.A. Qader, and G.R. Hill, Ind. Eng. Chem. Prod. Res. Develop. 9(3), 350-357 (1970).

Wu, W. and Haynes, H.W., Jr., Am. Chem. Soc. Div. Pet. Chem. Prepr., 20, 466 (175).

Yamadaya, S., M. Oba, and Y. Miki, Bull. Chem. Soc. of Japan, 50(1), 79-82 (1977).

CHAPTER III.

Experimental Apparatus and Procedure

1) Equipment

i) Introduction

The equipment used in the experimental program is shown schematically in Figure 3.1. The reactor system consists of three sections; the feed section, reactor section, and product recovery section. Except for the feed pumps, gas cylinders, and control panel, the unit was located in a walk-in hood having a 1.42 m^3/s exhaust fan and sliding safety glass windows. Gas cylinders, containing high purity hydrogen, nitrogen, and helium, were located outside the laboratory.

ii) Feed Section

Decalin used in this study was obtained from Matheson, Coleman, and Bell as a 98% pure mixture of cis and trans isomers. These isomers were separated by vacuum distillation to better than 90% purity for several studies. Tetralin was obtained from Aldrich Chemical Co. as a 99% pure compound and the fluorene used was also from Aldrich as 98% pure. These purities were confirmed by chromatographic anlaysis. The hydrocarbons were fed to the reactor system by means of a positive displacement Ruska pump having a 2.50×10^{-4} m^3 capacity which was driven by an explosion proof motor. The pumping rate could be varied from 5.56×10^{-10} to 6.67×10^{-8} m^3/s by changing the gears in the drive system. The pump cylinder was wrapped with a tape heater, insulated, and controlled by a Variac transformer to keep the feed above the temperature at which crystallization would occur. The temperature was monitored by a Doric

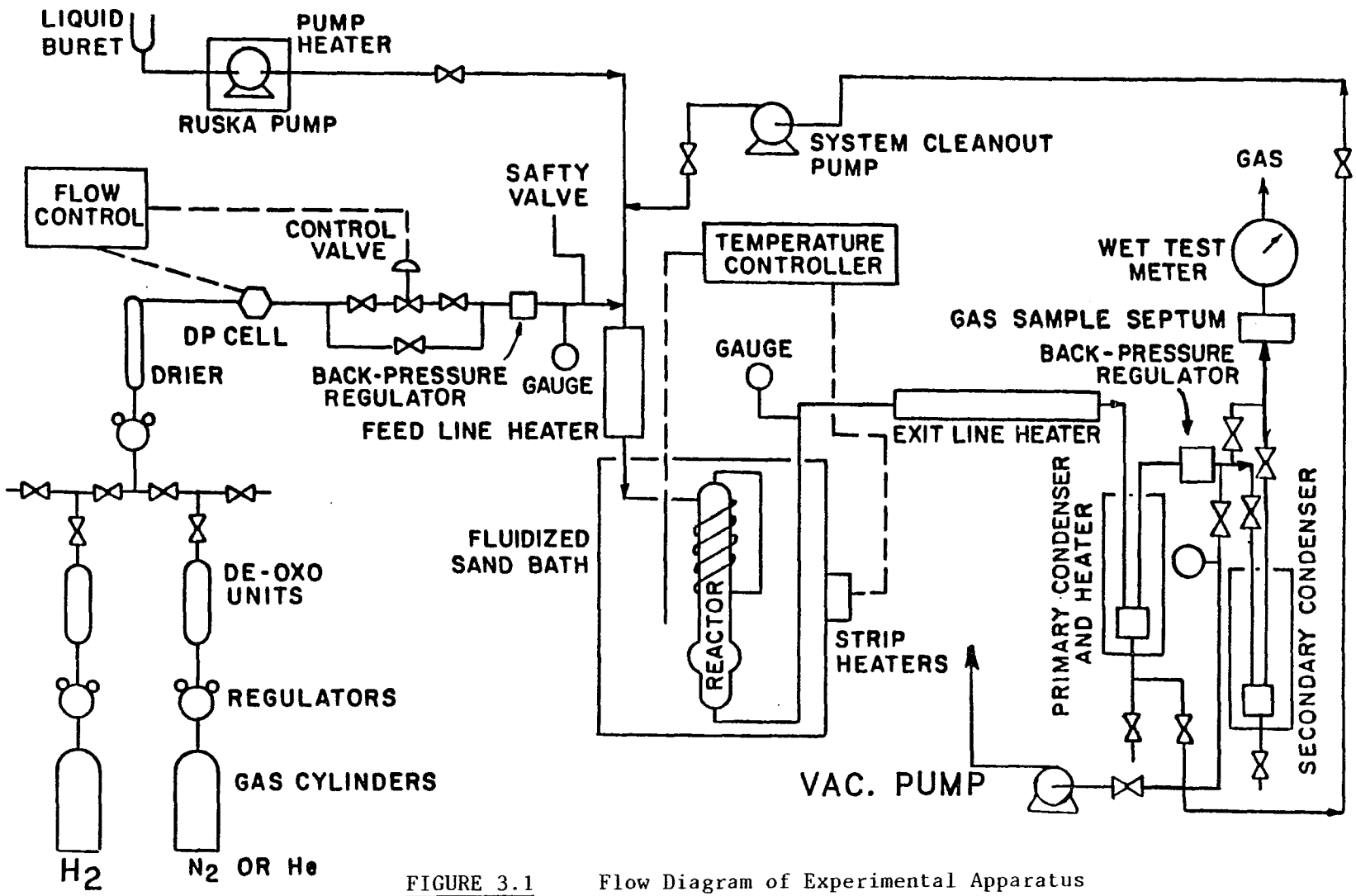


FIGURE 3.1 Flow Diagram of Experimental Apparatus

temperature indicator using an iron-constantan thermocouple and is accurate to ± 0.06°K. During a run, temperature was held to within ± 0.6°K of the desired setting.

Hydrogen supplied from a gas cylinder had any traces of oxygen present removed by passing it through a $Pd\text{-}Al_2O_3$ catalyst bed which converts O_2 to H_2O. The water formed is then removed in beds containing 3A molecular sieves and indicating Drierite desiccant. Hydrogen flow was regulated by a Research Controls, Inc. flow control valve coupled with an indicating flow controller located on the control panel. A Foxboro DP cell equipped with a 0.000152 meter integral orifice was used to measure hydrogen flow and provide an input signal to the flow controller. A Matheson pressure regulator set the supply pressure upstream of the control valve and a Mity-Mite back pressure regulator provided constant pressure downstream of the valve. All connections and lines were of 0.003175 and 0.00635 meter (1/8 and 1/4 inch) high pressure stainless steel tubing.

iii) Reactor Section

The reactor was a cylindrical fixed bed type and Figure 3.2 shows a detailed cross section of it in the sandbath vessel. The reactor is made from welded 0.0127 meter (1/2 inch) Schedule 80 Inconel pipe with a maximum capacity of 4.0×10^{-5} m^3. Glass wool was inserted first to fill the void space above the catalyst charge and to provide a region for the inlet gas to assume plug flow before contacting the catalyst. Another plug of glass wool was inserted to hold the catalyst in place. The reactor was sealed using a replaceable steel O-ring held by a temperature compensating coupling. The feed and product lines to and

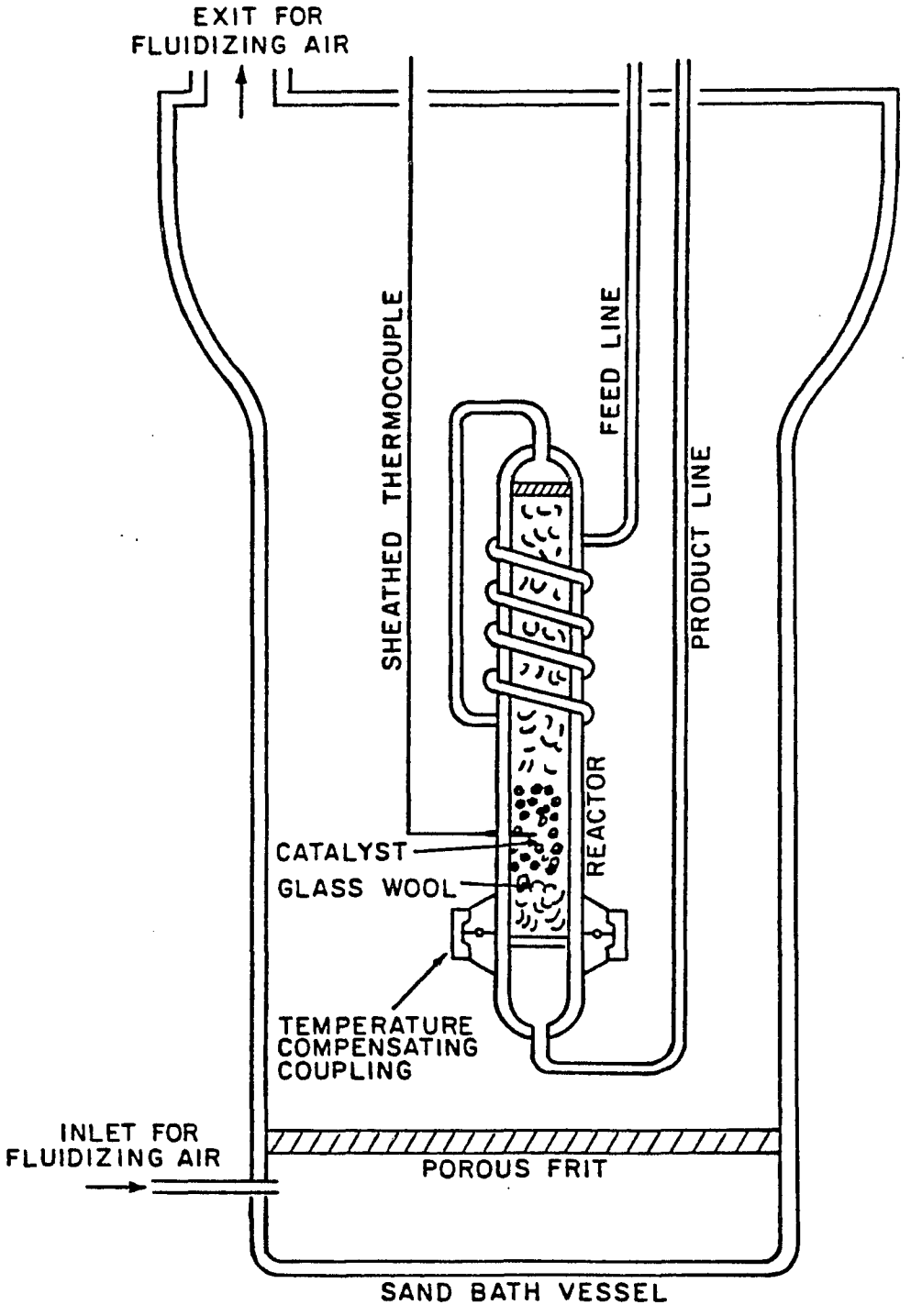


FIGURE 3.2 Detail of Reactor System

from the reactor were both heated by tape heaters, controlled by Variac transformers, and monitored with a Doric temperature indicator using iron-constantan thermocouples. These lines were heated to prevent crystallization and loss of fluorene in the system.

The hydrocarbon liquid and the hydrogen feeds were mixed in the heated feed line, vaporized, and brought to reaction temperature by flowing through a preheat coil in front of the reactor inlet in the sandbath. This section of the system was held at constant pressure by a Mity-Mite back pressure regulator downstream of the primary condenser. Pressure gauges were located at the reactor inlet and exit lines to monitor reactor pressure and in the event of excessively high or low reactor or sandbath air pressures, Mercoid pressure switches cut off the flow of feedstocks and power to the sandbath heaters. The whole system was protected by a 70 bar pressure relief valve.

iv) Product Recovery and Cleanout System

The reactor products were collected or sampled in the following manner. Upon leaving the heated exit line, the products passed through a condenser that was heated above the crystallization point of the fluorene/product mixture. The liquid condensate was collected and drained for analytical and material balance purposes. The product gas passed on through a dry ice/acetone condenser, which was bypassed except during material balance periods, where a second sample could be taken after warming to room temperature, and then through a fixed bed Rashing ring water saturator, and finally through a 0.001416 m^3 per revolution (0.05 ft^3/rev.) wet test meter to measure the volume. The exit gas was vented through the exhaust fan (equipped with an explosion proof motor)

to the atmosphere and sampled periodically for analysis from a septum located after the dry ice/acetone condenser. During a material balance period it was sampled after the wet test meter with a glass cylinder fitted with valves and a septum. Both methods gave the same molar composition of the gas.

In order to clean out the system between runs where a different feedstock was to be used, a centrifugal pump was run using the primary condenser as a reservoir for solvent. The pump line was connected to the Ruska pump, through the feed and product line, and back to the condenser where solvent was circulated for 1.08×10^4 to 1.44×10^4 seconds. A Sargent Welch vacuum pump was used to evacuate the system to remove residual solvent after clean out was completed.

2) Catalyst Preparation

The main catalyst used in this study was prepared in the Department using the metal loading technique from the Linde Molecular Sieve Catalyst Bulletin (1978). Other catalysts used were prepared in a similar manner.

1. A dilute solution of 0.02483 kgs of nickel nitrate hexahydrate ($Ni(NO_3)_2 \cdot 6H_2O$) from Aldrich Chemical Co. was added rapidly to an agitated slurry of 0.100 kgs of Linde LZ-Y62 zeolite catalyst powder in water. Physical properties of the zeolite catalyst are listed in Table 3.1.
2. The mixture was warmed on a hot plate with moderate vacuum applied to ensure that all air was removed from the catalyst pores.

TABLE 3.1 Linde LZ-Y62 Catalyst Properties (Linde Molecular Sieves, Zeolite Catalyst Data, Union Carbide Corp. 1978)

Surface Area, 1 point B.E.T.	9.48×10^5 m^2/kg
Unit Cell Size	24.73 Å
SiO_2	64.9 wt%
Al_2O_3	22.3 wt%
Na_2O	2.5 wt%
NO_3 -	0.4 wt%
$(NH_4)_2O$	9.8 wt%
Cl -	0.05 wt%
SiO_2/Al_2O_3, molar ratio	4.94
Na_2O/Al_2O_3, molar ratio	0.18

3. The slurry was agitated overnight, then filtered and washed with water to free the mixture of all soluble salts. A gravimetric analysis from Fritz and Schenk (1969) was performed on a sample of the catalyst to determine the percentage of nickel it contained.

4. The filter cake was finally dried overnight at 394°K to yield a free flowing powder.

5. Since the powder particle size was too small and might plug the reactor during a run, it was pressed into large wafers and then crushed and screened to a desired size before activation; 20/40 mesh (8.41×10^{-4} to 4.20×10^{-4} m) is the standard particle size used in all but the mass transfer studies.

6. The catalyst was placed in a quartz glass "boat" in a 0.051 meter O.D. quartz glass tube inside a horizontal electric oven. Air lines were connected to the entrance and exit of the tube.

7. An iron-constantan thermocouple was inserted through one end of the tube and rested in the catalyst bed to monitor the temperature on a Doric digital temperature indicator.

8. Air flow over the catalyst was begun as soon as heating started. The air was treated to remove any hydrocarbons by passing through a copper oxide catalyst bed at 811°K and subsequently dried by flowing through indicating Drierite.

9. The oven temperature was programmed as follows:

   a. Increase from ambient to 450°K at 0.0156°K/s.

   b. Hold at 450°K for 5.76×10^{4} s.

c. Increase from 450 to 811°K at 0.0193°K/s.

d. Maintain at 811°K for 1.08×10^4 s.

e. Cool and store in air-tight container with indicating Drierite desiccant.

10. Inert "mullite" (low surface area Norton No. 57 silica-alumina) was calcined in an open ceramic dish in a muffle furnace at 811°K for 8.64×10^4s. It was also stored in an air-tight container with Drierite desiccant.

Catalyst charges from previous runs were regenerated following steps 6 through 9 of the catalyst preparation procedure.

3) Run Procedure

i) Catalyst Reduction

The raw catalyst was weighed on a Mettler analytical balance and the desired amount (1.0×10^{-3} to 1.5×10^{-2} kgs) placed in the reactor with sufficient glass wool to fill the void space. A section of glass wool was inserted to hold the charge in place. The reactor was sealed using the temperature compensating coupling and a steel O-ring coated with copper compound to prevent it from sticking in the seal. The reactor was then pressure tested with nitrogen outside the sandbath to at least 1.5 times the desired run pressure and was then depressurized, bolted into the sandbath vessel and connected to the feed and exit lines. All connections were pressure tested before the tape heaters and insulation were added. The sandbath was subsequently heated to the desired reduction temperature (ex: 700°K) with hydrogen flowing at the desired run pressure (ex: 15.1 bar) through the catalyst bed overnight to reduce the oxide to metal.

ii) A Typical Experimental Run Procedure

1. After overnight reduction of the catalyst and then lowering of the reactor temperature from 700°K to the desired run temperature (ex: 661°K), the hydrogen flowrate was increased to 1.9 x 10^{-5} m^3/s (0.04 ft^3/min) or the desired rate by setting the automatic flow controller and back pressure regulators.

2. After about 1800 seconds for equilibration, the initial flowrate was measured with the wet test meter.

3. The hot supersaturated mixture of fluorene and decalin was charged to the heated Ruska pump (394°K) and any air in the pump purged manually.

4. The temperatures of the feed, exit, and condenser sections were set to prevent crystallization of the fluorene. Setpoints were 478°K for the feed and exit lines, 339°K for the primary condenser, and 195°K (dry ice/acetone bath) for the secondary condenser.

5. The Ruska pump was geared to the desired flow rate and turned on. Starting time was noted.

6. During the course of the run, gas and liquid samples were collected and analyzed by gas chromatography. Pressures and temperatures were also monitored and recorded.

7. For material balance calculations the hydrocarbon feedrate, exit gas flowrate, condenser liquid weights, and compositions were recorded. The material balance procedure is outlined in Appendix 2.

8. After obtaining the material balance data and product samples, the hydrocarbon feed was stopped. The samples were diluted in dichloromethane (DCM) if needed to prevent crystallization of fluorene at room temperature. The system was allowed to purge for 1800 seconds and the hydrogen flow rate was rechecked.

9. The system was then shut down and the cleanout system, if needed, put into operation while the catalyst charge was being regenerated or changed.

iii) Data Recorded

A sample data sheet for Run 82 is shown in Table 3.2. This record identifies the catalyst, the run conditions, and supplies basic material balance data. Units used in the sample data sheet are not consistent with the S. I. notation of the text, but represent the data as it was recorded in the laboratory. For the gas flow rate, the time for one revolution of the wet test meter 1.42×10^{-3} m^3 (0.05 cubic feet) is recorded in minutes. Condenser A is the primary heated condenser and Condenser B denotes the dry ice/acetone condenser.

4) Analytical Methods

i) Introduction

The majority of the analytical work was done by gas chromatography. This analysis was necessary for both material balances and kinetic data. The liquid feedstocks, liquid products, and gaseous streams were each analyzed for compound identification and molar or weight quantities. Initial identification was performed with an automated gas chromatograph/

TABLE 3.2

Run 82 Date 10/12/83 OPERATOR WDC

Catalyst Type: 2nd Batch NH_4Y/5%Ni
weight: 6.8108 + 0.1915 = 7.0023 gms.
volume: 17 cc
Previous Catalyst Use: Group V
Feedstock: 20% F/DEC

Desired Conditions:	T/°F	P/psig	cc/hr feed	min/rev gas
BASE	730	200	10	1.3

Barometric Pressure: 30.13 in Hg @ 76 °F Coke wt: 9.61%

Sample Number	Time on Feedstock/min.	Comments
1 A + B	92	First Washout
2 A + B	134	Second Washout
Dump Cond.	142.27	Start M.B.
MB Cond. A + B	204.06	Stop M.B.
-	234	Shutdown system

Actual Conditions: Gas Type: H_2
Initial gas rate 1.30 min/rev @ 79.5 °F
Final Gas rate 1.30 min/rev @ 82 °F

T/°F		P/psig		Run Purpose:
Feed Pump	230	cylinder	1100	recheck of Base Conditions
Feed line	394-420	line	550	
Reactor	730	Before CV	420	H_2 reduction for 860 min.
Sandbath	729	After CV	300	
Exit line	361	Reactor	205	
Condenser A	149	Condenser	205	
Condenser B	DI/ACE			
H_2 Line	339			

Material Balance Data: Tare wt/gms: A = 15.6210 B = in A

Time on oil/min	min rev	WTM °F	cc feed	React T/°F	SB T/°F	Press. psig	WTM ft^3	Prod Cond A,gm	Prod Cond B,gm
								24.0425	
142.27	1.29	83	65.45	730	729	205	0.00	-tare	None
204.06	1.29	83	75.98	730	729	205	2.40	8.4215	None

mass spectrometer system and the bulk of the remaining work was done with a gas chromatograph and recording integrator. The following sections describe the equipment and techniques for each analysis.

ii) Liquid Product Analysis

Liquid product samples were taken from the primary and secondary condensers during the experimental run and their respective weights and run duration times recorded. These samples were initially analyzed with a Finnigan 1020 Automated GC/MS System containing a feedback controlled chromatograph oven, an electron impact mass spectrometer, and a data system incorporating a Nova 3 computer, Perkin-Elmer disk drive, Tektronix 4006 CRT/keyboard terminal, Okidata printer/plotter, and a combined controller/interface. All entries were made via the CRT to the microprocessor. The GC/MS operating conditions and sample analysis data were stored on disks for retrieval and future use. The column used was a 6.10 meter by 3.175×10^{-3} meter (20 ft by 1/8 in) aluminum tube packed with 10% Silicone GE SE-30 on 60/80 mesh Chromasorb and the oven program was from 328 to 473°K with an initial time of 720 seconds, and a ramp rate of 0.2037°K/s, and a final time of 1920 seconds. Helium was used as the carrier gas at a rate of 5.0×10^{-7} m^3/s.

The separated compounds were then analyzed by the mass spectrometer to determine the identity of each by comparison with the National Bureau of Standards data on file. Once the identity of each compound was determined, the bulk of the product analysis was done using a dual column Perkin-Elmer model 990 gas chromatograph equipped with hot wire detectors. An identical column to that used in the GC/MS was used in the Perkin-Elmer GC with a matching oven program and helium as the carrier gas.

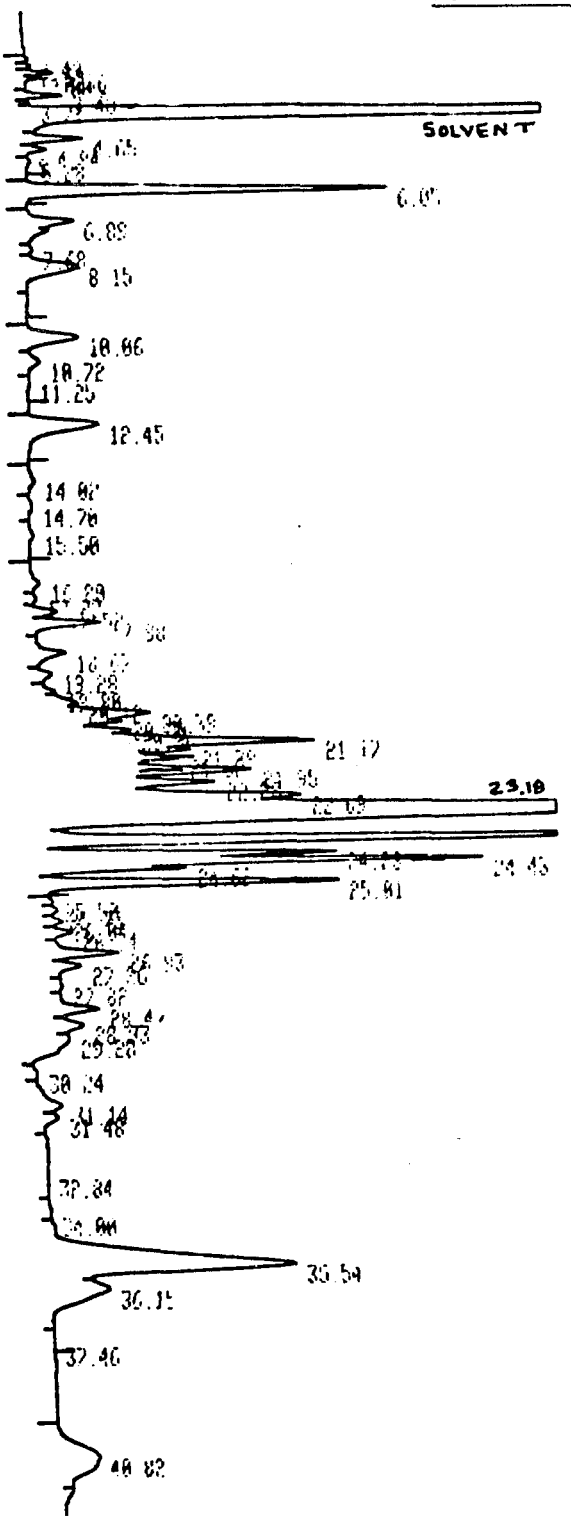
In order to determine the molar composition of each product sample, integration of the hot wire detector response peaks was carried out with a Hewlett-Packard model 3390 A integrator. Relative molar response (RMR) values obtained from Barry and Rosie (1971), Carson, Lege, and Young (1973), and by the molecular contribution method of Hougen, Watson, and Ragatz (1943) were used to convert areas to mole fractions. Adjusting these values by the respective molecular weights of the compounds also allowed the integrator to calculate weight fractions. These RMR values were checked on the GC by using an external standard made up of many of the products. These experimental results were found to be in agreement with the literature. Critical property data were obtained from Weast (1973) when needed and the method of calibration and the RMR values are presented in Appendix 1.

An example chromatogram from the H-P integrator for the liquid product of run 82 is shown in Figure 3.3 with corresponding response factors and weight percent distribution in Table 3.3. The use of the GC/MS provided for the initial qualitative analysis of samples and once each compound was identified, the Perkin-Elmer GC and H-P integrator served for the bulk of the quantitative analysis.

iii) Gas Product Analysis

Gaseous product samples were taken with either a gas-tight syringe from the septum located in the product line after the condensers or a glass cylinder fitted with valves on each end connected to the gas exit line. The gas cylinder was fitted with a septum so that samples could be analyzed immediately after a material balance period to prevent loss of lighter components with time. These samples were qualitatively

FIGURE 3.3 Run 82 Chromatogram Example



Retention Time/min.	Compound
2.86	isobutane
3.00	n-butane
3.48	2-methylbutane
4.65	2-methylpentane
4.94	3-methylpentane
6.05	methylcyclopentane
6.89	benzene
8.15	dimethylcyclopentane
10.06	methylcyclohexane
10.72	ethylcyclopentane
11.25	trimethylcyclopentane
12.45	toluene
14.02	dimethylcyclohexane
14.70	methylethylcyclopentane
15.50	dimethylcyclohexane
16.80	methylethylcyclopentane
17.58	xylene
17.88	xylene
18.67	xylene
20.39	mesitylene
21.17	dimethyloctahydro-pentalene
21.39	mesitylene
21.62	dimethyloctahydro-pentalene
21.95	mesitylene
22.28	dimethyloctahydro-pentalene
22.69	mesitylene
23.18	trans-decalin
23.86	cis-decalin
24.23	methyl indan
24.43	methyl indan
24.62	tetralin
25.01	naphthalene
25.50	dimethyl indan
25.73	dimethyl indan
26.04	dimethyl indan
26.34	dimethyl indan
26.93	methyl naphthalene
27.82	methyl naphthalene
28.47	biphenyl
28.93	ethylene bis-benzene
29.28	dimethyl naphthalene
30.24	dimethyl naphthalene
31.14	methyl biphenyl
31.48	methyl biphenyl
35.54	fluorene
36.15	methyl biphenyl
40.82	methyl fluorene

TABLE 3.3 Run 82 Example Liquid Product Distribution

Retention time/min	Area	Response Factor	wt% Product	Compound
2.86	23197	.80016	0.130	isobutane
3.00	12275	.81106	0.069	n-butane
3.48	33642	.86866	0.203	2-methylbutane
4.65	54035	.90923	0.344	2-methylpentane
4.94	17164	.92704	0.110	3-methylpentane
6.05	490800	.93689	3.188	methylcyclopentane
6.89	77018	1.00000	0.534	benzene
8.15	140900	1.02380	1.000	dimethylcyclo-pentane
10.06	114030	1.04740	0.828	methylcyclohexane
10.72	26286	.99761	0.182	ethylcyclopentane
11.25	2302	1.06720	0.017	trimethylcyclo-pentane
12.45	183700	1.02580	1.306	toluene
14.02	14509	1.06720	0.107	dimethylcyclo-hexane
14.70	9633	1.06720	0.071	methylethylcyclo-pentane
15.50	11170	1.06720	0.083	dimethylcyclo-hexane
16.80	17631	1.06720	0.130	methylethylcyclo-pentane
17.58	35014	1.04540	0.254	xylene
17.88	98802	1.04540	0.716	xylene
18.67	67265	1.04540	0.488	xylene
20.39	223110	1.02570	1.586	mesitylene
21.17	496180	1.15070	3.958	dimethyloctahydro-pentalene
21.39	199190	1.02570	1.416	mesitylene
21.62	202640	1.15070	1.616	dimethyloctahydro-pentalene
21.95	448810	1.02570	3.191	mesitylene
22.28	308400	1.15070	2.460	dimethyloctahydro-pentalene
22.69	486090	1.02570	3.456	mesitylene
23.18	4304600	1.11140	33.164	trans-decalin
23.86	1024900	1.11140	7.896	cis-decalin
24.23	327680	1.12510	2.556	methyl indan
24.43	510250	1.12510	3.980	methyl indan
24.62	127330	1.12830	0.996	tetralin
25.01	354330	1.17750	2.892	naphthalene
25.50	5910	1.17200	0.048	dimentyl indan
25.73	17136	1.17200	0.139	dimethyl indan
26.04	24172	1.17200	0.196	dimethyl indan
26.34	46594	1.17200	0.379	dimethyl indan
26.93	142100	1.17350	1.156	methyl naphthalene
27.82	70960	1.17350	0.577	methyl naphthalene
28.47	180060	1.19570	1.493	biphenyl
28.93	127390	1.21740	1.075	ethylene bis-benzene

Table 3.3 Continued.

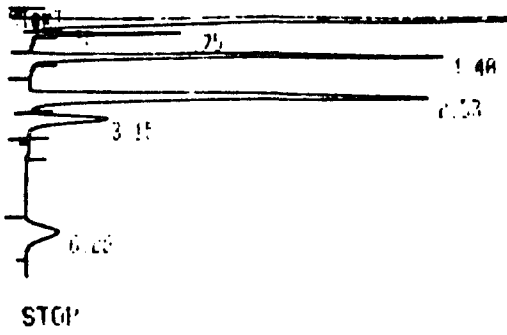
Retention time/min	Area	Response Factor	wt% Product	Compound
29.28	142490	1.19530	1.181	dimethyl naphthalene
30.24	8285	1.19530	0.069	dimethyl naphthalene
31.14	85439	1.21740	0.721	methyl biphenyl
31.48	52594	1.21740	0.444	methyl biphenyl
35.54	1065400	1.18540	8.754	fluorene
36.15	255850	1.21740	2.159	methyl biphenyl
40.82	281380	1.37470	2.681	methyl fluorene

analyzed using external standards on a Carle Series S Analytical Gas Chromatograph connected to a Hewlett-Packard 3390 A integrator. Once the identity of each compound was determined with pure gases obtained from Matheson, the quantitative analysis for mole fractions was made on the Perkin-Elmer model 990 GC using the same conditions as with the liquid analysis except for the oven temperature which was held constant at 328°K. The column used was 1.83 meters of 3.175×10^{-3} meter (6 ft by 1/8 inch) stainless steel tube packed with Chemipack C-18/100 mesh obtained from Alltech Associates, Inc. Integration of the hot wire detector response areas was performed with a H-P 3390 A integrator and RMR values obtained from Barry and Rosie (1971) normalized the area percent values to mole fractions. An example of the H-P integrator output for the product gas analysis of run 82 is shown in Figure 3.4 with corresponding response factors and hydrogen-free mole percentages in Table 3.4. For material balance calculations, the area counts were referenced to a standard sample of isobutane in helium as shown in Appendix 1 in order to determine the total fraction of hydrocarbons contained in the gas. Table 3.5 gives the detailed operating conditions of the Perkin-Elmer GC for both gas and liquid analysis.

iv) Coke Determination

In order to determine the degree of coking present in the reactions, the used catalyst was dried at 450°K, weighed, and regenerated by burning off the coke at 811°K in air following steps 6 through 9 of the catalyst preparation procedure. The catalyst was then reweighed and the difference giving the amount of coke built up on the catalyst during a run period. Several samples were boiled under reflux

FIGURE 3.4 Run 82 Gas Product Chromatogram Example



Retention time/min	Compound
0.75	ethane
1.40	propane
2.53	isobutane
3.15	n-butane
6.25	2-methylbutane

TABLE 3.4 Run 82 Example Hydrogen Free Gas Product Distribution

Retention time/min.	Area	Response Factor	Hydrogen Free Mole % Product	Compound
0.75	806	1.7240	6.539	ethane
1.40	4806	1.3699	30.984	propane
2.53	8272	1.1490	44.730	isobutane
3.15	1991	1.1490	10.766	n-butane
6.25	1577	9.4060E-01	6.981	2-methyl-butane

TABLE 3.5 Detailed Operating Conditions
Perkin-Elmer 990 Gas Chromatograph

Parameter	Liquid Analysis	Gas Analysis
He rate/m^3/s @ 7.45 bar	5.00×10^{-7}	5.00×10^{-7}
Manifold T/°K	523	523
Injector T/°K	573	573
Initial T/°K	328	328
Final T/°K	473	328
Ramp Rate/°K/s	0.2037	None
Initial Time/s	720	None
Final Time/s	1920	Hold
Hot Wire Detector		
Temp./°K	523	523
Current/mA	225	225
Injection Size/m^3	1.0×10^{-9}	1.0×10^{-6}

in toluene to check for hydrocarbons on the used catalyst but none were found by chromatographic analysis. Therefore, the difference in weight between the dry and regenerated catalyst was used to determine the amount of coke accumulated by the catalyst in a run period. It should be noted that this analysis neglects oxidation of the catalyst in the calculation of weight % coke.

v) Safety Considerations

Since the hydrocracking reactions were carried out in the presence of hydrogen gas at elevated temperatures and pressure, the following special precautions (Bryant, 1966) were taken to ensure safe operation.

1. Circuit breakers were located immediately outside the door for all power supplies.
2. The exhaust fan equipped with an explosion proof motor was operated at all times during experimentation with the safety glass panels closed down except for space to allow for an upward draft.
3. Gas cylinders were located outside the building.
4. Quick shut off valves were located outside the hood near the emergency exit.

5) Literature Cited

Barry, E.F. and D.M. Rosie, J. Chromatogr., 59, 269-279 (1971).

Bryant, P.A., "Hydroisomerization of Normal Pentane over a Zeolite Catalyst", Ph.D. Dissertation, L.S.U., 38-40 (1966).

Carson, J.W., G. Lege, and J.D. Young, J. of Chromatographic Science, 11, 503-508 (1973).

Fritz, J.S. and G.H. Schenk, Jr., Quantitative Analytical Chemistry, 2nd ed., 511-513 (1969).

Hougen, Watson, and Ragatz, Chemical Process Principals, Part 1, Material and Energy Balances, 87-91 (1943).

Linde Molecular Sieves Catalyst Bulletin, "Ion Exchange and Metal Loading Procedures", Union Carbide Corporation.

Weast, Robert C., ed., Handbook of Chemistry and Physics, 54th ed., CRC Press, Cleveland (1973).

CHAPTER IV.

Discussion of Experimental Results

1) Overview of Experimental Work

The purpose of this chapter is to present the results of the laboratory experiments that were performed during the course of this study. Conclusions are drawn in this discussion based on interpretation of the experimental results with application of the quantitative results reserved for the next chapter where the kinetic model is developed. The results are presented in chronological order by run number through run 61, after which the data is grouped by experimental series.

i) Development of Quantitative Results

Based on previous experimental work on the reactor system used in this study, a program was initiated to study the hydrocracking of coal-derived liquids using fluorene as a model compound. Starting with the work of Bryant (1966) and continuing to date by many investigators, it has been shown that the reactor system under study behaves essentially as a plug flow integral reactor with isothermal operation easily maintained for long time periods.

The first twelve runs used this system without the present modifications to attempt to react fluorene, phenanthrene, and acenaphthene using 3-methylpentane as a solvent on a ZSM-5 (Union Carbide ELZ-105-6) type catalyst at 589°K and 4.5 bar. No reaction was noted with this system as the solute concentrations were small (<1%) and difficult to analyze. Runs 13 through 18 were under the same conditions concentrating on the fluorene/3-methylpentane feedstock without success. The solubility of these polynuclear aromatics was quite low in

3-methylpentane so a more suitable solvent (1-methylnaphthalene) was used in runs 19 through 23. No reaction was noted until run 22 when 5% Ni was added to the ZSM-5 type catalyst. 1-Methylnaphthalene was observed to be reactive, but fluorene, at 10 weight % of the feedstock, was not converted. Temperatures ranged from 589 to 700°K.

At this point, the vacuum pump and solvent cleanout pump systems were added to the unit and the feed and exit lines were heated and insulated to prevent the loss of fluorene and heavier products in the lines. The need for a hydrogen rich solvent was concluded from the previous runs and decalin was chosen as a practical grade mixture of 40 % trans- and 60 % cis-isomers. Pure isomers were not required as it was found that each contributed to the reaction system without negative side effects. Decalin isomers and 5 weight % fluorene in decalin were fed to the system in runs 24 thru 27 from 644.3 to 700°K in hydrogen on the 5% Ni/ZSM-5 catalyst and although no fluorene reaction was observed, the cis- isomer of decalin was found to react.

The possibility of purely thermal reactions occurring and masking the catalytic effects was checked in run 28 with inert "mullite" in the reactor starting at 478°K increasing to 789°K over a 3.0×10^4 s time period with samples analyzed every 3600 s as temperature increased. Although the G.C. analysis technique was not completed at the time of this run, area % analysis of the product showed that no reaction occurred as no "peaks" were shown on the integrator output other than the feedstock and the area under these curves did not change. Therefore, thermal reactions were not present in the range of conditions of this study. This observation was checked by two other quantitative runs in the space-time results section 3.

In the preceding runs, no fluorene reaction was noted so a Y zeolite catalyst study was begun in run 29 with a Ru loaded Y type. Dehydrogenation of cis-decalin was observed, with tetralin and naphthalene being the primary products. Through run 34, this was the only reaction observed with a small amount of BTX also produced.

Runs 35 through 37 tested the use of cyclohexane as a possible hydrogen donor solvent but it was found to have too low a boiling point and caused pluggage of the reactor system by fluorene. Therefore, light compounds were discarded as possible solvents.

The final set of runs before quantitative work, used a 5% Ni on Y zeolite (Union Carbide LZ-Y62) catalyst prepared in the laboratory. The catalyst was found to be highly reactive to decalin/fluorene feedstocks but not useful when methylcyclohexane or 1-methylnaphthalene were solvents for fluorene. There were still problems associated with G.C. analysis of the small concentrations of fluorene and reaction products, so the feed pump was heated and a 20 weight % mixture of fluorene in decalin was studied in runs 48 through 52. No reaction occurred at 589°K, however from 644 to 661°K both decalin and fluorene conversions were observed, with the identification of indanes (2,3-dihydroindenes) and biphenyls confirmed by GC/MS analysis. All other products were identified at this point by GC/MS and by comparison with known samples.

The results of runs 53 through 58 confirmed the previously observed reaction of cis-decalin and fluorene and the lack of conversion of the trans-decalin isomer. Runs 59 through 61 established the ability to regenerate the catalyst to high activity and during these runs, the gas and liquid sample analysis procedure was incorporated in the material balance routine so that quantitative work could be done. Hydrogen was

used as the carrier gas in all runs except for number 59 where helium was used to determine the role of hydrogen. There was some conversion of decalin observed; however, fluorene did not react. The same catalyst was used in run 60 without regeneration and although conversion of both decalin and fluorene was found, it was much less than had been observed in previous runs. The catalyst was badly coked from the helium experiment and therefore it was concluded that the use of hydrogen was essential to reduce coke formation so that reaction sites would be available for fluorene hydrogenation to occur.

Starting with run 64, the primary catalyst of the study was prepared and used for the remainder of the work. Ion exchange of $Ni(NH_3)_2 \cdot 6H_2O$ was performed on the Y zeolite base material yielding a catalyst of higher activity than the previously used $NiCl_2$ exchanged catalyst. After run 64, minor changes in the product recovery system were made to improve sample collection and enhance the analytical results. These changes did not alter the previous results, but did increase the reliability of the material balance method. All the material balances were performed by the final method developed and described in Appendix 2. It should also be noted that the catalyst was changed and regenerated after each run in all other experimental work presented in these results except for the tetralin runs (62 and 63) and three of the fluorene/decalin ratio runs (69,70, and 71) which are basically qualitative in nature and not affected by the repeated exposure of the catalyst without regeneration.

ii) Quantitative Results and Material Balance Method

The remainder of the experimental runs (62-124) are presented in chronological order in Appendix 3. The following sections of this

chapter present the results grouped by experimental series, for example, temperature series, pressure series, etc. All process variables are held constant except for the variable of interest in the series, which is varied from the base conditions determined from the qualitative work. Data for each run was accepted based on the C and H balance closure results as described in Appendix 2. If the C balance was less than 90%, indicating a loss of products in the system lines, the run data was rejected from the experimental series and the conditions repeated in another run if necessary.

The base run conditions are listed in Table 4.1 as the average of runs 93, 94, 95, and 114. Components of the product distribution of these runs were grouped together for analysis as shown in Appendix 2 and listed in Table 4.2. This component grouping into 14 species by parent structure simplified the reaction structure without altering the general scheme of the reaction network developed in the next chapter. Shown in Figure 4.1 is the feedstock free product distribution for the base runs as mole percent. The conversion of each feedstock is listed in Table 4.3 for the base runs. Tetralin is not included in Table 4.3, but was found in the feedstock (~1.0 wt%). This data shows that feedstock conversion is high while yielding the primary products for fuel stocks (BTX, alkanes, and cyclopentanes) and other products suitable for recycle as solvent if desired.

As a comparison of donor solvents with decalin, tetralin was used in runs 62 and 63 to investigate its interactions with fluorene and the catalyst. Fluorene conversion was not significantly improved over its conversion in decalin and the primary products were naphthalenes from tetralin dehydrogenation with less of the desired gasoline fractions

TABLE 4.1

Average Base Run Conditions

Catalyst:

5% Ni on LZ-Y62 zeolite

7.005×10^{-3} kg weight

1.3×10^{-5} m^3 volume

Feedstock:

Feedrate = 2.842×10^{-9} m^3/s at 394°K.

31.31 wt % trans-decalin

48.21 wt % cis-decalin

1.05 wt % tetralin

19.43 wt % fluorene

Reactor conditions:

Temperature = 661°K.

Pressure = 14.8 bar

Molar gas density = 0.269 kg-mole/m^3

Space-time = 4.8 s.

Superficial gas velocity = 1.38×10^{-2} m/s

Feed/catalyst ratios:

H_2/hydrocarbon = 41.8 kg-mole/kg-mole

H_2 feedrate = 7.131×10^{-7} kg-mole/s at 300°K

Gas rate during

mat'l balance = 7.175×10^{-7} kg-mole/s at 301°K

Average material balance closure:

Carbon closure = 94.36 %

Hydrogen closure = 98.95 %

TABLE 4.2

Compound Group Code Names and Number Assignments

Compound Group	Code Name	Structure Type
1	ALK	alkanes (gas)
2	CPT	cyclopentanes
3	CHX	cyclohexanes
4	BZ	benzenes (BTX + mesitylenes)
5	ABZ	alkylbenzenes (more sub. than BZ group)
6	DMOHP	dimethyloctahydro-pentalene
7	TD	trans-decalin
8	CD	cis-decalin
9	TT	tetralin
10	IN	indanes
11	NAP	naphthalenes
12	BIP	biphenyls
13	FL	fluorene
14	MFL	methylfluorene

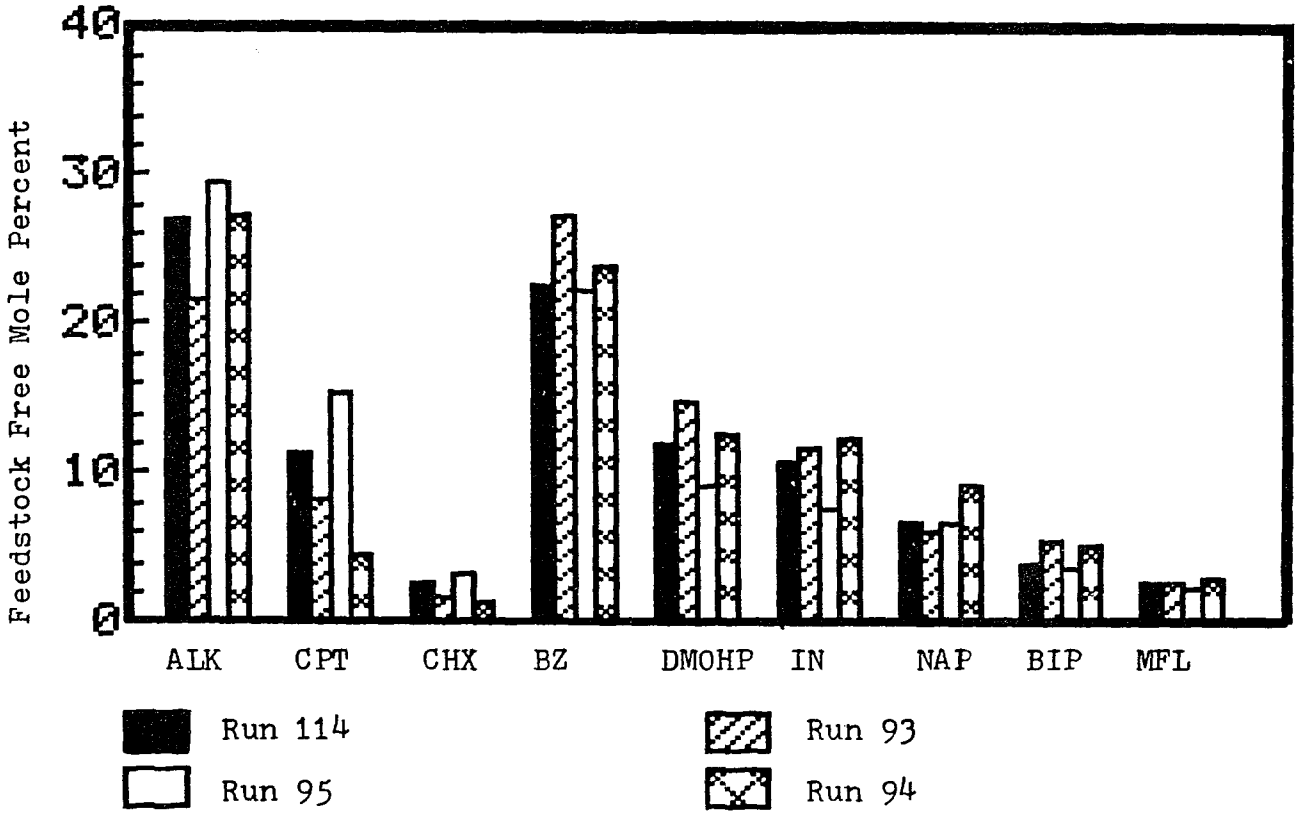


FIGURE 4.1 Feedstock Free Product Distribution of Base Runs

TABLE 4.3

Base Run Feedstock Conversions

	% Conversion		
Run	fluorene	trans-decalin	cis-decalin
93	49.2	-7.1[a]	78.1
94	75.5	25.5	91.1
95	69.6	9.4	86.7
114	59.3	2.9	89.1
Average	63.4	7.7	86.3

a: negative indicating formation and not conversion.

formed as shown in Figure 4.2. Should recycle of the solvent be desired, decalin would be more acceptable than tetralin as initial feed because its products are hydrogen rich and would not require as much hydrotreating as naphthalene would before recycle.

2) Thermal and Transport Limitations

i) Thermal Limitations

As discussed above, no thermal reactions were observed for run 28 at typical process conditions for 5 % fluorene in decalin from 478 to 789°K. This experiment convered the range of temperatures used in the study to ensure that no thermal reactions were masking catalytic effects. A qualitative plot of area % of the products vs. temperature is shown in Figure 4.3. No other products were observed except the feedstock components. This qualitative result is due to the fact that the analytical and material balance procedures were not completed at the time of the run. However, a material balance would not change the results, as no reaction was found.

ii) Transport Limitations

In heterogeneous catalysis with porous solid catalysts, there are seven steps involved (Froment and Bischoff, 1979):

a. Transport of reactants from the main stream to the catalyst pellet surface.
b. Transport of reactants into the catalyst pores.
c. Adsorption of reactants on the sites.
d. Surface chemical reaction.
e. Desorption of products.
f. Transport of products out of the pores to the surface.

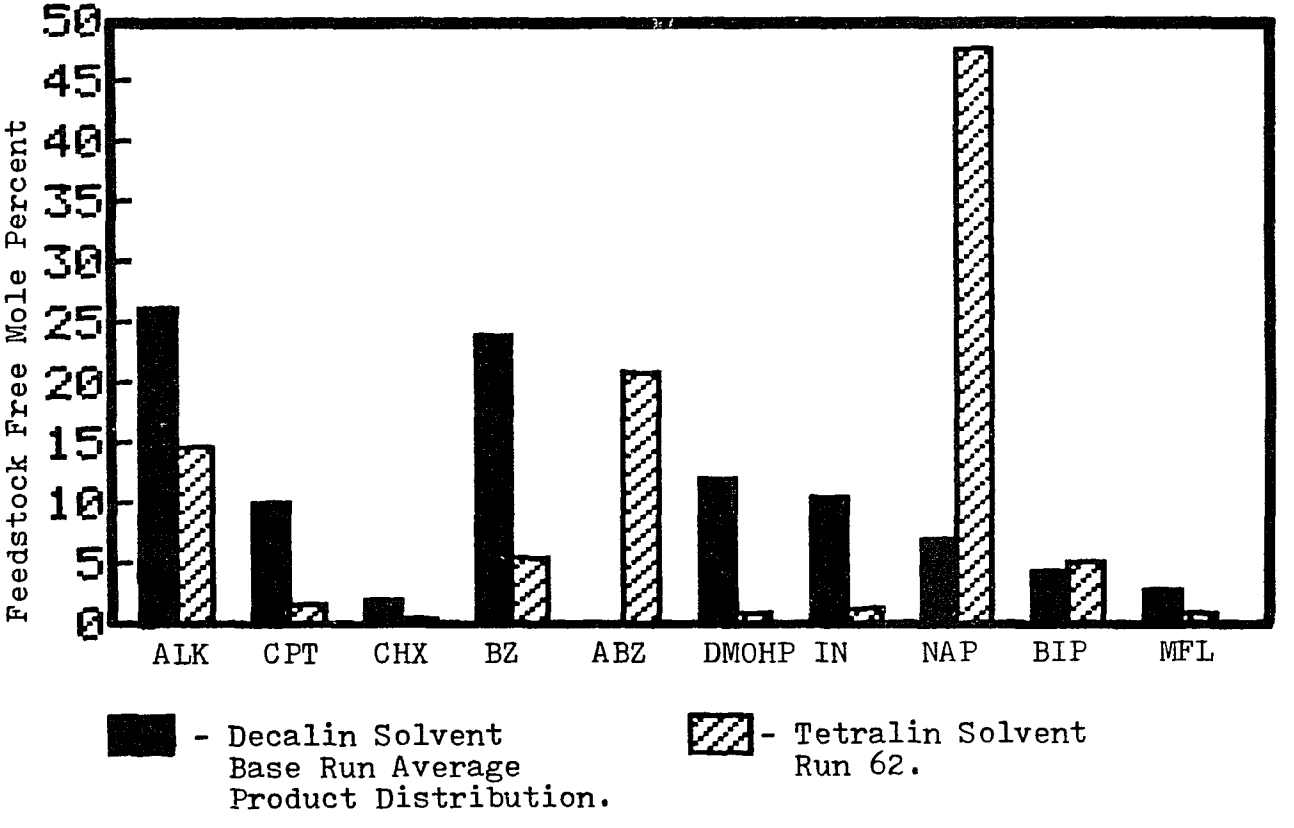


FIGURE 4.2 Comparison of Decalin and Tetralin as Donor Solvents. A Feedstock Free Product Distribution.

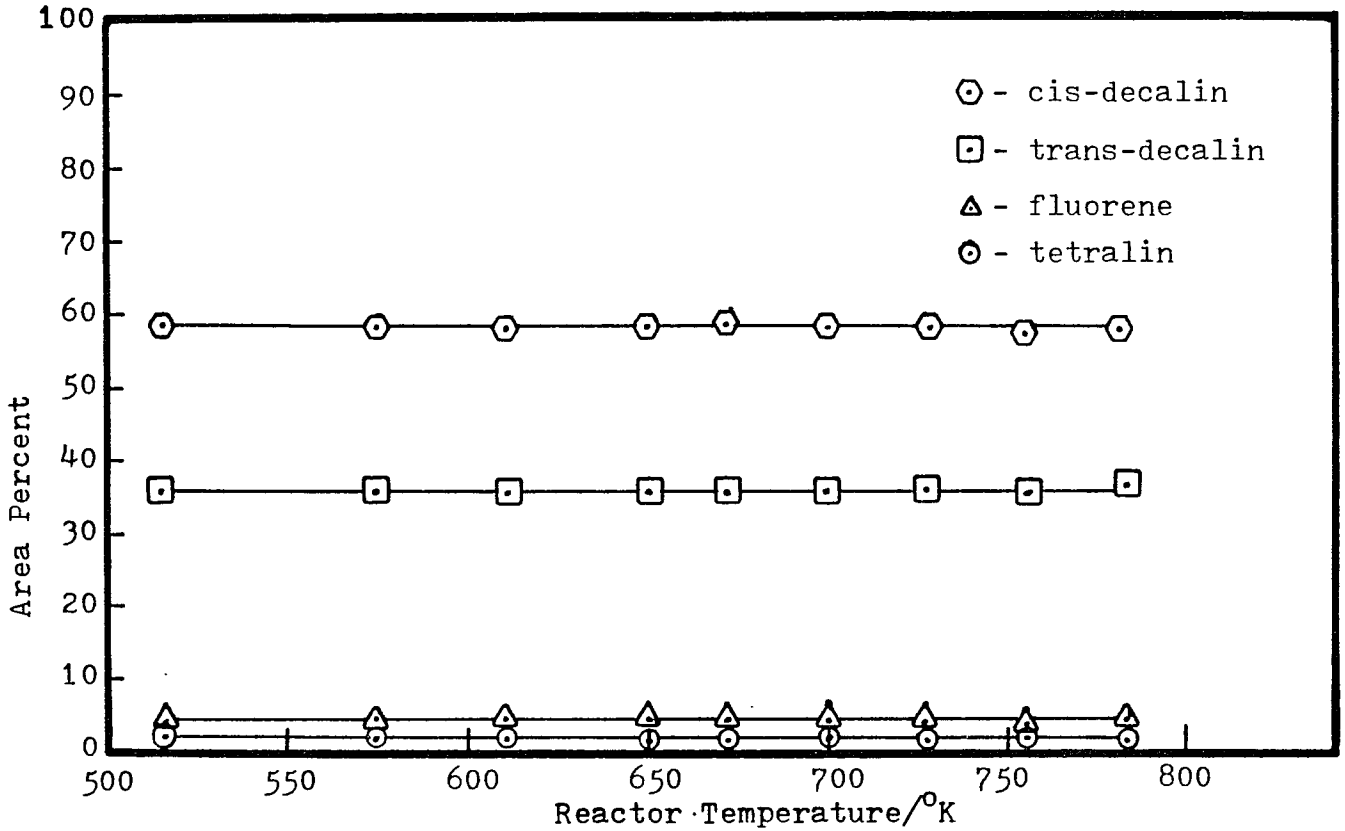


FIGURE 4.3 Test for Thermal Reactions in Run 28 w/o Catalyst

g. Transport of products from the surface back to the main fluid stream.

To study the surface phenomena (steps c,d, and e) of the reaction system, the transport effects must be accounted for before proceeding.

An evaluation of the effects of mass transfer was made by making a series of runs with varying gas velocities while maintaining other process conditions constant. These runs are summarized in Table 4.4, and a plot of conversion vs. superficial gas velocity is shown in Figure 4.4. As can be seen, the conversions were not strongly affected by the gas velocity. If fluid-to-catalyst particle mass transfer had been a limiting step in the process, the higher velocity run would have shown a significantly higher conversion than observed at the lower gas velocities. These runs indicate that mass transfer is not limiting within the range of velocities employed in this study.

Most of the catalyst surface area is located in the interior of the particles as the wall area of the pores. This interior surface area cannot be utilized unless the reactants and products are continuously transferred into and out of the pores. Because of chemical reaction in the interior of the catalyst, concentration gradients are established in the pores that cause mass transfer to occur by means of diffusion. Depending on the conditions, the diffusion may be ordinary, Knudsen, or configurational.

Due to the finite rate at which diffusion occurs, the concentration of reactants is lower in the particle interior, with the result that the average reaction rate will be somewhat lower than if there were no mass transfer step. However, if the surface reaction step is much slower than the pore diffusion step, concentration gradients will be small and

TABLE 4.4

Summary of Gas Velocity Run Conditions for
Effect of External Mass Transfer

Operating Conditions:

Feedstock: 20 wt % fluorene in decalin isomers

Catalyst: 5 % Ni on LZ-Y62 zeolite, 20/40 mesh

Pressure: 14.9 bar

Temperature: 661°K

H_2/HC ratio: 42 kg-mole/kg-mole

Run[a]	Gas Vel/ m/sx10^3	Cat Wt/ kgx10^3	Cat Vol/ m^{3}x10^6	HC feedrate/ m^3/sx10^9	space-time/s
121	7.3	3.5608	6.7	1.421	4.7
BASE	13.8	7.0046	13.0	2.842	4.8
119	20.1	11.131	21.8	4.547	5.5

a: Detailed data may be found in Appendix 3.

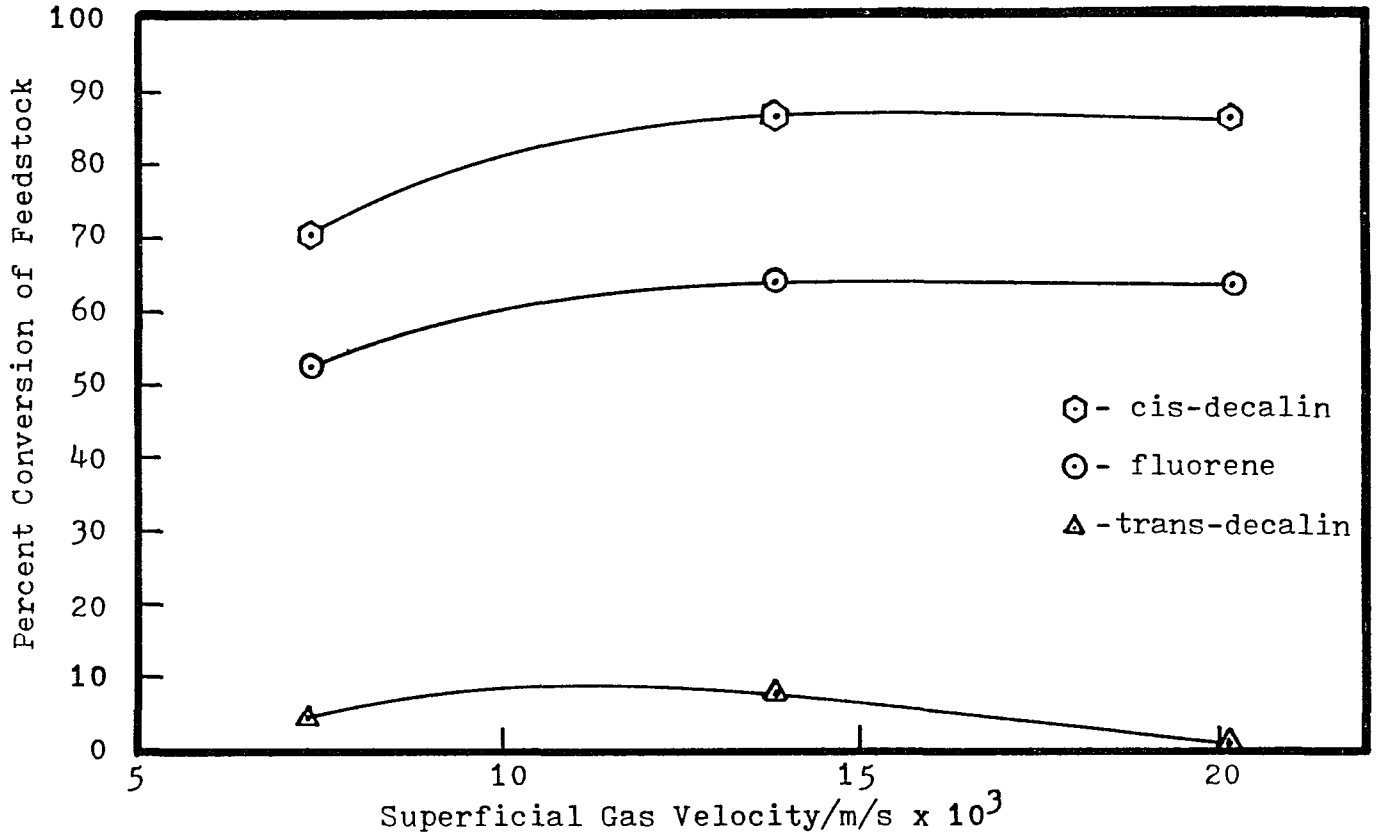


FIGURE 4.4 Test of External Mass Transfer Limitations at 661°K and 14.8 Bar.

the reaction rate will not be significantly affected. Conversely, when surface reactions are fast with respect to the pore diffusion rates, the actual reaction rates will be much lower than those calculated using the bulk stream compositions.

As a measure of pore diffusion limitations, an effectiveness factor, η, defined as the ratio of the observed reaction rate to that which would occur without concentration gradients was estimated assuming Knudsen diffusion was operative, which may or may not be the actual conditions. From Satterfield (1980), η can be related to the reaction conditions through a modified Thiele modulus Φ, defined as:

$$\phi = \frac{Rp^2 x(\text{Experimental reaction rate})}{D_{eff}\ C} \qquad 4.1$$

where for base conditions:

Rp = average particle radius, 5.0×10^{-5} m

D_{eff} = effective diffusivity, 1.97×10^{-8} m^2/s

Experimental reaction rate = experimentally observed average consumption of key component fluorene at base conditions, 1.1×10^{-3} kg-moles/$m^3 \cdot$ s, increased one order of magnitude to represent an upper bound on the rate.

C = concentration of fluorene at outside of particle surface, 104.1×10^{-5} kg-mole/m^3

The effective diffusivity of fluorene in the catalyst is estimated by:

$$D_{eff} = 97(Rr)\ \frac{\varepsilon}{\lambda}\ (T/M)^{\frac{1}{2}} \qquad 4.2$$

with the physical properties:

Rr = pore radius, 4.0×10^{-10} m

ε = porosity of catalyst, 0.51

λ = tortuosity, 2.0

T = temperature, 661°K.

M = molecular weight of fluorene, 166.23 kg/kg-mole

For the indicated conditions, a value of Φ of 0.13 was calculated. As discussed by Hill (1977), an analytical relationship can be developed between the effectiveness factor and the Thiele modulus. For values of the modulus less than 1.0, the effectiveness factor is essentially unity, while for large values the effectiveness factor is inversely related to the modulus. In other words, since η approaches unity as Φ approaches zero, it can be seen that the reaction does not appear to be limited by pore diffusion.

The above result is at best a rough approximation of the effectiveness factor, therefore it was felt that the limitations of pore diffusion should be experimentally verified. This is conventionally done by changing the catalyst particle size while maintaining all other conditions. If pore diffusion is significant, the decrease in particle size will be accompanied by an increase in the conversion of the reactants. Two particle size distributions (4.20×10^{-4} to 8.41×10^{-4} m and 1.80×10^{-4} to 2.50×10^{-4} m) were tested at 661 to 633°K for typical run conditions as summarized in Table 4.5. As shown in the bar graphs of Figure 4.5, no significant changes in conversion of the feedstock components was found. Therefore, pore diffusion was not found to be rate limiting under the conditions of the experimental study. Should configurational diffusion be present, which cannot be measured by conventional methods, the rate of reaction in the pores would be negligible, and the rate coefficients would be based upon the external surface area of the particles.

TABLE 4.5

Summary of Catalyst Particle Run Conditions for Effect of Pore Diffusion

Operating Conditions:

Feedstock: 20 wt % fluorene in decalin isomers

Feedrate: 2.84×10^{-9} m^3/s

Catalyst: 5 % Ni on LZ-Y62 zeolite

Pressure: 14.8 bar

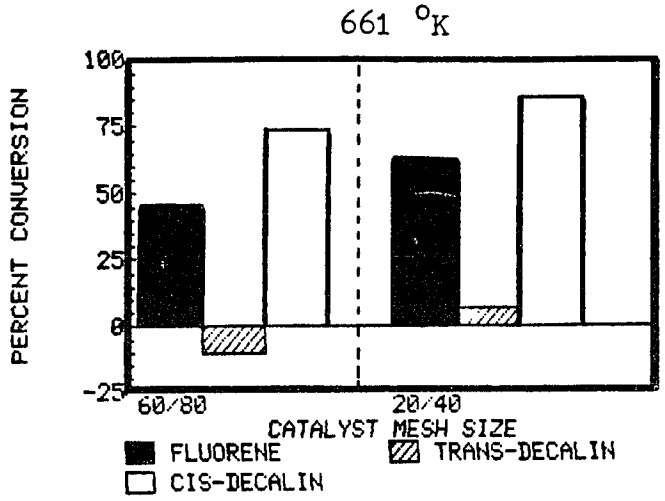
Temperature: 633 and 661°K

H_2/HC ratio: 42 kg-mole/kg-mole

Catalyst particle size distributions/m x 10^4:
4.20 to 8.41 (20/40 mesh)
1.80 to 2.50 (60/80 mesh)

Run[a]	Particle size dist./ m x 10^4	Temp. °K	Cat Vol/ m^3 x 10^6	space-time/s
BASE	4.20 to 8.41	661.0	13.0	4.8
118	1.80 to 2.50	660.2	13.0	4.8
108	4.20 to 8.41	632.8	13.2	5.1
120	1.80 to 2.50	633.0	12.8	4.8

a: Complete run data is found in Appendix 3.



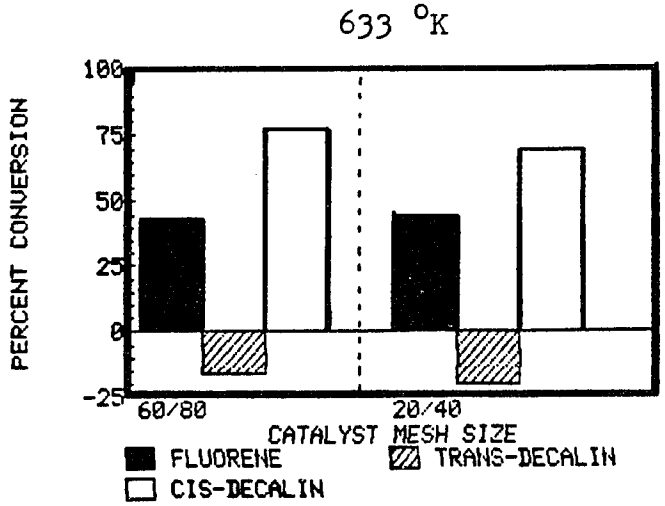


FIGURE 4.5 Test of Pore Diffusion Limitation at 661 and 633°K for 5 % Ni on LZ-Y62 Zeolite.

In summary, the results of the transport and thermal studies have shown that for the conditions investigated, neither external mass transfer nor pore diffusion affect the rate of reaction and the reaction is not masked by thermal cracking, although configurational diffusion may cause some reactions to occur on the exterior surface. It is safe to assume therefore, that the results obtained in this study reflect the interactions at the catalyst surface or catalyst exterior.

3) Effect of Space Time and Temperature

i) Space Velocity Series

A composite reaction scheme for the catalytic hydrocracking of fluorene and decalin from previous work was presented in Chapter II. The simplest way to investigate all the reaction paths possible is to vary space-time (catalyst volume/feedrate at reaction conditions) in the integral reactor at otherwise constant conditions and observe the changing product distributions. Such a study comprises a considerable part of the discussion presented in Chapter V. One reason for obtaining this type of experimental data is that one is able to observe the yields of reaction products and intermediates as they change concentration with space-time. This provides insight into the nature of the reaction scheme and mechanism. Another reason for investigating the effect of space-time is that only this type of information can be used to evaluate a proposed kinetic model.

For an integral reactor of the type used in this study where reactant concentrations varied considerably from the entrance to the exit, it was necessary to integrate the rate equations to obtain a relationship between concentration and time. A more direct way is to

determine numerical derivatives of conversion vs. space-time with the gradient at each space velocity being proportional to the reaction rate at that particular composition and temperature. However, very accurate data are required to obtain a fair estimate of the reaction rates. Therefore, the integral method was chosen and applied to the data presented here. Development and application of the integral method is presented in Chapter V for the following experiments.

Space time was varied from 0 to 5 s by changing the catalyst volume in each run at 663 and 661°K maintaining other conditions constant using a feedstock of 20 weight % fluorene in decalin isomers. The runs used and conditions during them are summarized in Table 4.6. In each run, the catalyst used was 5% Ni on Y zeolite, which was changed and/or regenerated after each experiment. Concentration vs. space-time for the compound groups was taken from the material balance results and is shown in Table 4.7 for the 633°K series and in Table 4.8 for the 661°K series. For the runs where space-time equals zero, inert "mullite" was used to fill the void space in the reactor. Also note that the zero space-time runs showed essentially no reaction, further reinforcing the fact that no thermal reactions are occurring in the system.

ii) Temperature Series

The effect of temperature is an important measure of the performance of a reactor system. The selectivity and control over the desired products may be largely influenced by the reactor temperature and must be accounted for in the reaction kinetics.

For homogeneous systems, the rate expression for a simple reaction of:

$$A \xrightarrow{k} B$$

TABLE 4.6
Summary of Space-time Run Conditions at 633 and 661°K.

Operating Conditions:

Catalyst: 5 % Ni on LZ-Y62 zeolite, 20/40 mesh

Feedstock: 20 wt % fluorene in decalin isomers

Feedrate: 2.84×10^{-9} m^3/s

Pressure: 14.8 bar

Molar gas density/kg-mole/m^3:

0.281 at 633°K and 0.269 at 661°K

Superficial gas velocity/m/s:

1.33×10^{-2} at 633°K and 1.39×10^{-2} at 661°K

H_2/HC ratio: 41.8 kg-mole/kg-mole

Run[a]	Space-time/s	Temp./ °K	Cat Wt/ kg x 10^3	Cat Vol/ $m^3 \times 10^6$
101.1	0.0	633.2	0.0	0.0
110	4.5×10^{-1}	632.8	0.5073	1.2
112	7.5×10^{-1}	633.7	1.0000	2.0
109	9.3×10^{-1}	633.7	1.0004	2.4
111	1.6	633.2	2.0011	4.2
113	3.1	633.2	4.1300	8.1
108	5.1	632.8	7.0071	13.2
101	0.0	660.9	0.0	0.0
104	3.6×10^{-1}	660.9	0.5026	1.0
102	9.2×10^{-1}	660.9	1.0006	2.5
105	1.6	660.9	2.0012	4.3
103	2.4	660.9	3.0014	6.6
BASE	4.8	661.0	7.005	13.0

a: Detailed data may be found in Appendix 3.

TABLE 4.7

Concentration Function of Space-time at 633°K.

Space-time/s	Compound Group Conc./kg-mole/m^3 x 10^5						
	ALK	CPT	CHX	BZ	DMOHP	TD	CD
0.0	0.0	0.0	0.0	0.6	0.2	227.0	356.7
0.45	8.9	2.7	0.8	11.2	5.3	213.9	293.2
0.75	13.3	2.1	0.7	10.6	4.7	244.5	339.0
0.93	22.1	2.0	0.9	26.7	16.7	229.1	234.4
1.6	36.3	12.8	3.3	45.5	23.7	253.7	242.0
3.1	50.8	20.3	5.3	86.0	61.3	253.3	90.0
5.1	54.7	23.9	6.4	80.0	54.6	246.9	100.7

Space-time/s	Conc./kg-mole/m^3 x 10^5					
	TT	IN	NAP	BI	FL	MFL
0.0	8.4	1.2	1.4	6.5	108.7	0.0
0.45	6.5	1.6	4.2	9.1	100.4	2.7
0.75	8.1	5.9	14.1	23.9	109.1	4.1
0.93	-	15.5	13.5	17.4	82.0	6.7
1.6	7.3	9.5	13.4	18.3	84.1	8.2
3.1	7.8	28.9	22.0	25.3	63.8	8.0
5.1	7.5	26.8	19.1	24.1	65.2	10.2

TABLE 4.8

Concentration Function of Space-time at 661°K.

Space-time/s	Compound Group Conc./kg-mole/m^3 x 10^5						
	ALK	CPT	CHX	BZ	DMOHP	TD	CD
0.0	0.0	0.0	0.0	0.6	0.2	217.0	341.7
0.36	18.3	5.1	1.6	14.0	10.2	206.1	233.0
0.92	30.9	10.7	4.9	19.6	12.3	225.7	252.9
1.6	43.0	17.4	3.8	29.2	14.6	203.4	205.0
2.4	107.9	40.4	10.1	74.6	32.2	216.8	133.1
4.8	115.3	45.2	10.5	102.1	50.7	186.7	42.8

Space-time/s	Conc./kg-mole/m^3 x 10^5					
	TT	IN	NAP	BI	FL	MFL
0.0	8.1	1.2	1.4	6.2	104.1	0.0
0.36	6.3	13.0	11.7	9.4	73.4	5.1
0.92	6.3	13.1	12.5	11.5	65.2	5.4
1.6	4.9	9.7	18.1	12.7	51.6	7.5
2.4	6.9	32.2	23.3	14.2	38.0	8.4
4.8	6.0	44.6	30.7	19.0	38.2	11.4

may be expressed as:

$$r_A = k(T)\ f(\text{concentration}, T) \qquad 4.3$$

where k(T) is in consistent units depending on the concentration terms to give the rate as kg-mole/$m^3 \cdot s$. A similar form of the rate expression may be assumed for heterogeneous systems, i.e., a pseudo-homogeneous rate expression wherein the rate constant, k, includes the catalyst parameters provided there are no transport limitations as was previously discussed. For a given catalyst, this is a valid simplifying step to aide in analysis where the reaction scheme is complex and little is known about the adsorption and desorption steps around the surface reaction.

This does not, however, eliminate the temperature dependency of the rate constant, which is a misnomer, as the rate "constant" is only constant for a given temperature assuming other reactor conditions are maintained. For many reactions and particularly elementary reactions where the rate expression coresponds to a stoichiometric equation, the temperature dependent term, k, has been found to be well represented by the Arrhenius law:

$$k = A\ e^{-E/RT} \qquad 4.4$$

where:

A = frequency factor, assumed independent of T, with units of k.

E = apparent activation energy, kcal/kg-mole.

R = gas constant, 1.987 kcal/kg-mole°K.

T = temperature, °K.

Therefore, the rate constant is a function of temperature with the activation energy and frequency factors being constant for a given reaction model. The usual procedure then is to plot the ln of k vs. 1/T to yield the activation energy from the slope (-E/R). Experimentally, this would involve obtaining concentration vs. space-time data over the temperature range of the study to produce a typical Arrhenius plot.

Since little was known about the effect of temperature on the reaction scheme of fluorene and decalin combined, a wide range (a 10°K increase in temperature typically doubles the reaction rate) of temperature data was required to determine processing conditions. Therefore, product concentration data was obtained from 622 to 694°K at one space-time maintaining all other conditions at base for a 20 weight % fluorene feedstock. This data is used in conjunction with the base (661°K) temperature/space-time data in a pattern search routine to determine E and A and is tested with the 633°K space-time data for the model as presented in Chapter V. The run results are summarized in Table 4.9 listing the conversions for each feedstock and concentration vs. temperature data is listed in Table 4.10.

Overall conversion trends show an initial increase in fluorene conversion up to about 650°K, after which little increase is indicated. Cis-decalin conversion indicates the same trend and trans-decalin appears to be formed at low temperatures and then consumed at higher temperatures. this was also observed by comparison of the 633°K to the 661°K space-time runs indicating a possible equilibrium reaction being established between the two isomers.

An overall indication of the effect of temperature on selectivity can be made by comparison of the feedstock free product distributions on

TABLE 4.9

Conversion of Feedstocks as a Function of Temperature

Run[a]	T/°K	% Conversion		
		fluorene	trans-decalin	cis-decalin
106	622.6	41.3	-16.6	64.1
108	632.8	44.4	-19.7	69.3
76	639.5	72.5	1.0	78.0
78	649.8	78.2	7.2	88.7
79	655.4	78.0	14.5	90.9
BASE	661.0	63.4	7.7	86.3
77	667.0	84.8	16.6	90.6
75	672.6	63.6	3.9	74.0
73,96	677.7	64.7	4.9	77.4
98[b]	683.5	73.9	20.9	90.3
97	688.2	85.1	21.5	77.9
99	694.5	71.9	11.2	70.1

a: Detailed run data may be found in Appendix 3.

b: M.B. closure marginal.

TABLE 4.10

Concentration of Compound Groups as a Function of Temperature.

	Compound Group Conc./kg-mole/m^3 x 10^5						
T/°K	ALK	CPT	CHX	BZ	DMOHP	TD	CD
622.6	37.1	14.2	4.3	71.0	48.3	242.4	118.9
632.8	54.7	23.9	6.4	80.0	54.6	246.9	100.7
639.5	118.7	41.8	10.7	105.2	51.2	210.9	73.2
649.8	159.1	47.1	13.8	123.2	57.9	194.8	36.3
655.4	181.5	65.8	16.1	108.3	48.3	168.3	27.6
661.0	115.3	45.2	10.5	102.1	50.7	186.7	42.8
667.0	241.4	53.1	12.1	113.4	44.7	171.8	29.8
672.6	118.1	40.0	7.7	82.8	32.4	187.4	79.3
677.7	161.2	37.7	8.1	83.7	34.5	189.4	70.0
683.5	192.8	29.7	6.8	84.8	38.3	147.0	28.1
688.2	266.0	46.1	8.0	127.9	19.0	154.6	67.6
694.5	158.1	16.0	4.2	77.7	24.6	167.7	87.9

	Conc./kg-mole/m^3 x 10^5					
T/°K	TT	IN	NAP	BIP	FL	MFL
622.6	6.8	18.7	17.7	21.0	69.4	9.0
632.8	7.5	26.8	19.1	24.1	65.2	10.2
639.5	8.5	37.6	25.4	18.2	30.7	11.1
649.8	7.6	43.8	27.2	20.5	24.0	9.5
655.4	6.0	42.0	31.1	17.1	22.8	10.3
661.0	6.0	44.6	30.7	19.0	38.2	11.4
667.0	6.4	54.7	39.6	17.2	16.5	8.0
672.6	6.2	43.0	30.0	16.1	37.2	11.6
677.7	6.0	44.2	37.6	17.2	38.4	15.0
683.5	6.0	55.2	44.9	20.5	27.6	13.0
688.2	3.2	40.0	48.5	19.3	16.7	6.7
694.5	3.4	36.1	39.9	17.2	30.2	14.5

a mole percentage basis since the feedstock composition for each temperature run is essentially the same. These percent distributions are shown in Figures 4.6, 4.7 and 4.8 indicating an increase in the Group 1 (alkanes) compounds with a drop in Group 6 (dimethyloctahydropentalene, DMOHP) and little effect on the other products except for Group 2 (cyclopentanes) which increases up to a temperature of about 660°K and then drops off. An increase in gas production with a decrease in DMOHP verifies that: a) the severity of hydrocracking increases with temperature and b) DMOHP is an intermediate product formed as an isomer of decalin that is cracked to cyclopentanes which increase and then crack to produce more hydrocarbon gas.

4) Effect of Feed Ratios

In order to apply the results of the study to commercial operations, where changes in feedstock composition, recycle of donor solvents, and adjustment of processing conditions may occur to achieve a desired product distribution, the effect of feed ratios on the kinetics must be resolved. Two ratios were varied in this study; the ratio of fluorene to decalin obtained by changing the weight % of fluorene over the range of 0 to 20 % in decalin and the ratio of hydrogen to total hydrocarbon feedstock (both decalin and fluorene) obtained by changing the liquid pump feedrate over the range of 6.92×10^{-10} to 5.68×10^{-9} m^3/s at an average pump temperature of 392°K. All other processing conditions were held essentially constant. A summary of the run conditions with the reference run numbers is shown in Table 4.11.

Fluorene concentration was not increased over 20 % to avoid line pluggage and the hydrogen to hydrocarbon mole ratio ranging from 21 to 174 was just within operating limits of the reactor system. Within these

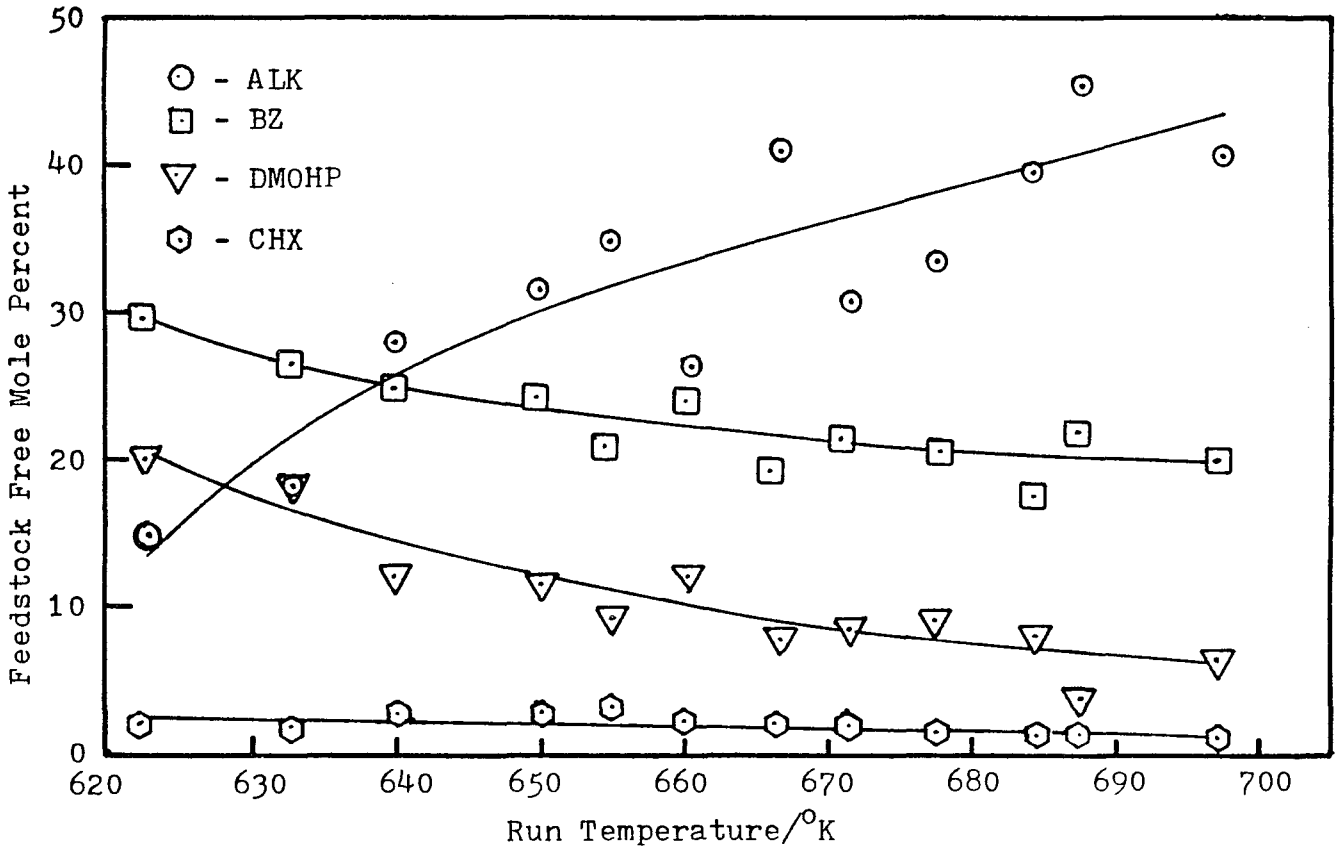


FIGURE 4.6 Effect of Temperature on Feedstock Free Product Distributon (Alkanes, Benzenes, DMOHP, and Cyclohexanes only, see Figure 4.7 and 4.8 for other product distributions).

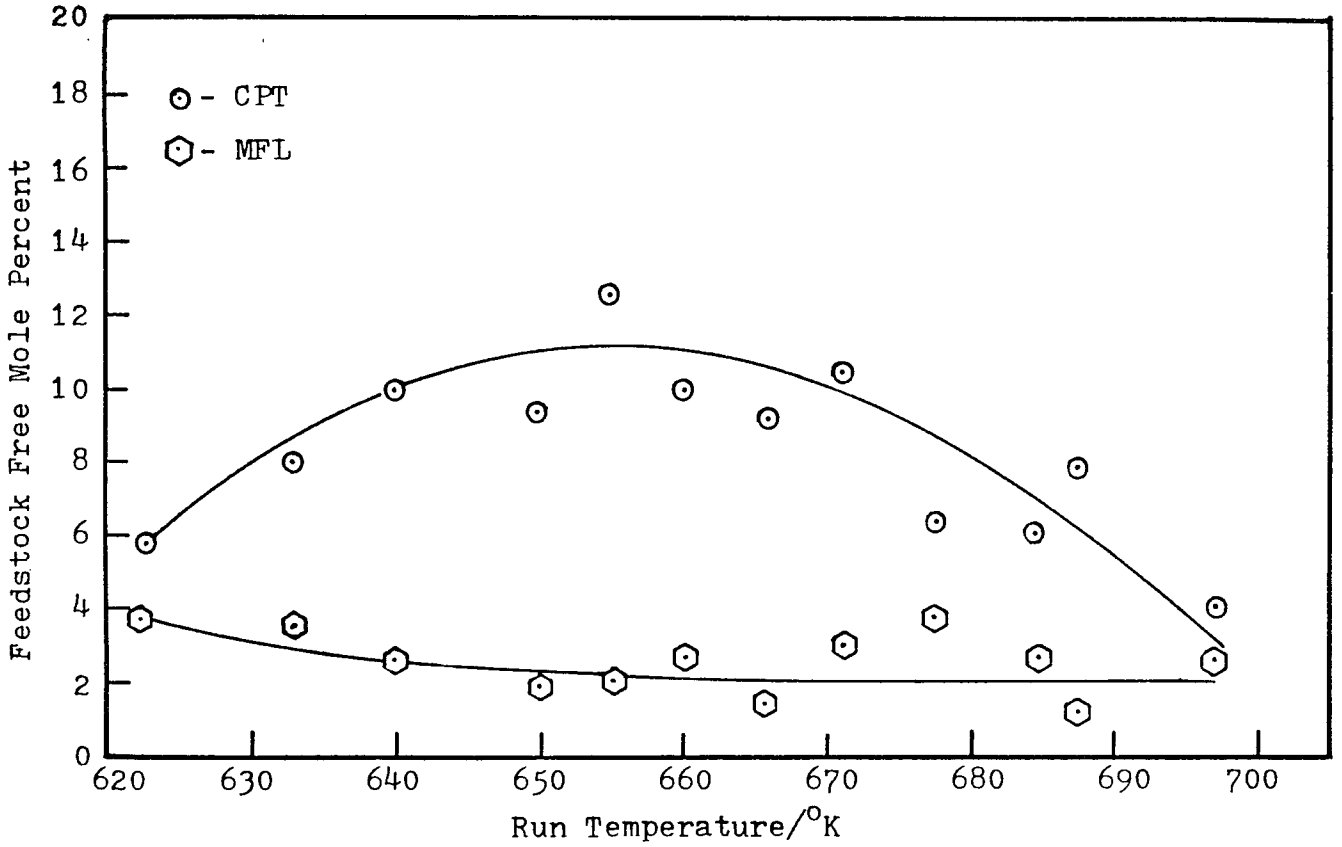


FIGURE 4.7 Effect of Temperature on Feedstock Free Product Distribution (Cyclopentanes and Methyl fluorene only, see Figure 4.6 and 4.8 for other product distributions).

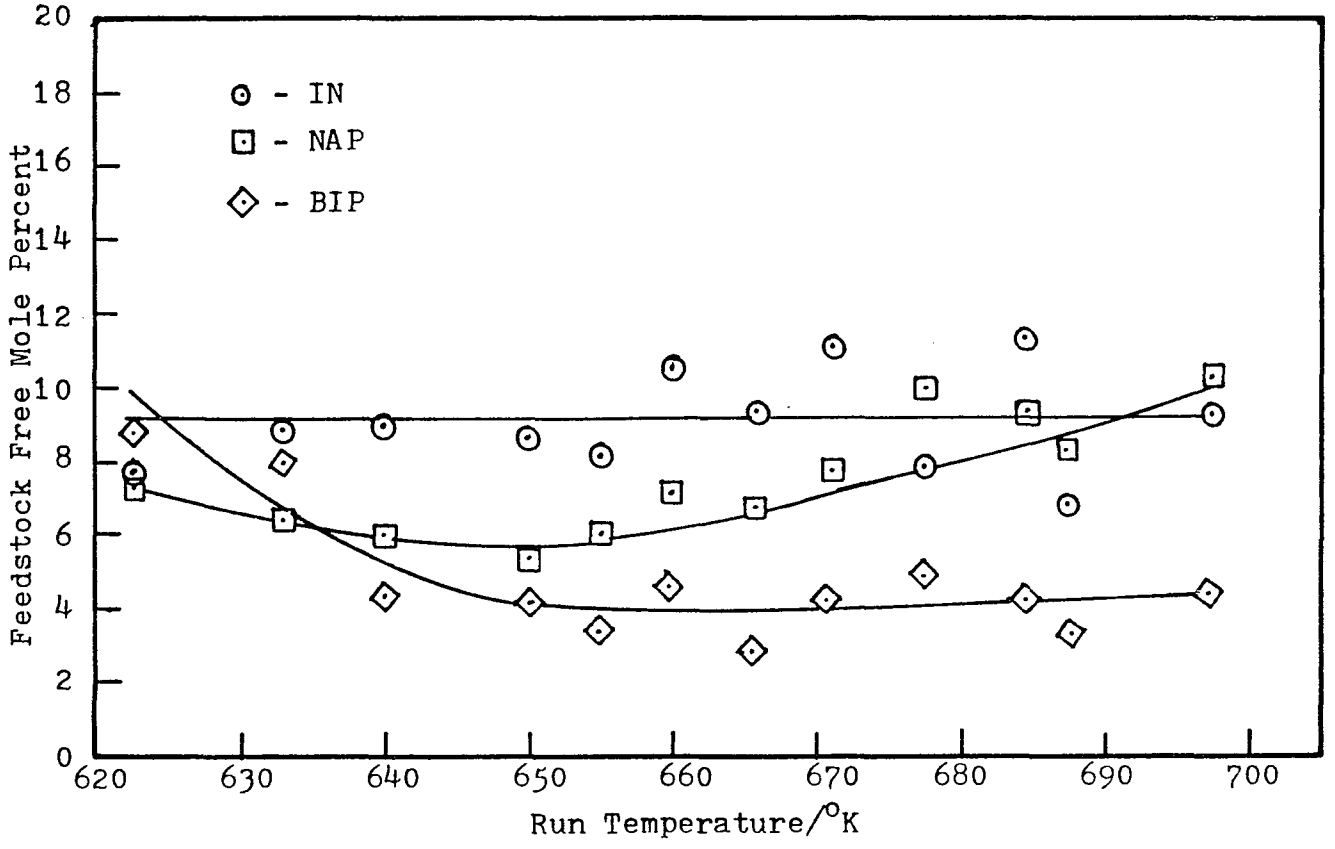


FIGURE 4.8 Effect of Temperature on Feedstock Free Product Distribution (Indanes, Naphthalenes, and Biphenyls only, see Figure 4.6 and 4.7 for other product distributions).

TABLE 4.11

Summary of Feed Ratio Series Run Conditions

Operating Conditions:

Catalyst: 5% Ni on LZ-Y62 zeolite, 20/40 mesh.

wt = 7.000×10^{-3} kg

vol = 1.3×10^{-5} m^3

Pressure: 15.1 bar

Temperature: 661°K

H_2 Feedrate: 7.13×10^{-7} kg-mole/s

Run[a]	% fluorene in decalin	H_2/HC ratio	Hydrocarbon feedrate/ $m^3/s \times 10^9$	Space-time/s
100	0.1	42.1	2.838	4.8
69	5.1	40.7	2.841	5.0
70	9.5	41.2	2.844	4.9
71	14.6	41.2	2.840	5.0
BASE	19.4	41.8	2.842	4.8
85	22.4	173.8	0.697	4.9
84	22.4	84.9	1.422	4.8
BASE	19.4	41.8	2.842	4.8
87	20.2	26.0	4.547	4.7
88	20.2	21.1	5.683	4.7

a: Detailed run conditions may be found in Appendix 3.

limitations, changing the feed ratios establishes two points of insight into the reaction. First, changing the ratio of fluorene to decalin should indicate interactions between the model compound and solvent and secondly, varying the amount of hydrogen present in the reactor compared to the hydrocarbon mixture should show the contribution of the carrier gas to the reaction mechanism.

i) Effect of Fluorene/Decalin Ratio

The experimental results of the hydrocarbon ratio study are shown in Table 4.12 as concentration of each compound group for the % fluorene in the feedstock. Although trends are not consistent in all compound groups due to scatter of the data, several important observations are made. As the fluorene concentration in the solvent increases, the alkanes, cyclopentanes, and cyclohexanes concentrations decrease along with an increase in decalin isomers, biphenyls, and fluorenes. This indicates the alkanes, cyclopentanes, and cyclohexanes are products of decalin alone and that fluorene takes up reaction sites and shifts the decalin reaction more toward dehydrogenation than cracking. These two paths for decalin are shown to exist as both cracked products and dehydrogenated ones are formed with pure decalin as a feedstock. The shift in the decalin reaction away from cracked products by the presence of fluorene also indicates that these two components are closely linked in the reaction scheme and that for the fluorene reaction to proceed, decalin must be included. Except for DMOHP, which is assumed to be an isomer of decalin, all other products which show uncertain trends or no change and are therefore possible products of both model compound and solvent. This represents then a complex network between decalin and fluorene.

TABLE 4.12

Experimental Results of Fluorene/Decalin Ratio Series as a Function of % Fluorene

% fluorene in decalin	Compound Group Conc./kg-mole/m^3 x 10^5												
	ALK	CPT	CHX	BZ	DMOHP	TD	CD	TT	IN	NAP	BIP	FL	MFL
0.1	234.1	124.4	24.1	146.7	54.4	99.7	10.9	0.0	59.9	32.3	5.0	1.6	0.0
5.1	328.7	91.3	20.9	97.6	36.5	176.7	26.6	0.3	56.0	28.9	3.5	1.4	1.0
9.5	203.4	47.7	13.0	66.5	33.1	242.7	94.5	0.0	49.7	27.3	6.4	8.1	5.5
14.6	147.7	27.3	8.1	43.6	23.7	255.2	186.3	6.9	28.3	24.4	9.9	29.0	0.0
19.4	115.3	45.2	10.5	102.1	50.7	186.7	42.8	6.0	44.6	30.7	19.0	38.2	11.4

The conversion of each feedstock is shown in Table 4.13 as a function of % fluorene in the feedstock. As fluorene percentage increases, trans-decalin is no longer consumed, but produced from cis-decalin, again indicating a shift in the decalin reaction away from cracking and toward isomerization. Cis-decalin maintains a fairly constant conversion level except for the 15% run. As was earlier discussed, the catalyst had been used in two previous runs (5 and 10 % fluorene of this series) without regeneration as these runs were made before the procedure of change and regeneration after every run was begun. Even in light of this problem, it does not change the trends indicated in Table 4.12 or 4.13.

ii) Effect of Hydrogen/Hydrocarbon Ratio

The results of this series are shown in Table 4.14 and Table 4.15 as concentration of products and conversion of feedstocks respectively. In Table 4.14, the concentrations are listed with decreasing hydrogen/hydrocarbon ratio (H_2/HC). All concentrations increase uniformly as the ratio decreases without any obvious deviations noted, indicating that relative selectivity is not signficiantly changed. Further indication of the selectivity not changing is shown in Table 4.16 by expressing the distribution of products as feedstock free mole percent with decreasing hydrogen/hydrocarbon ratio. Except for the first run (H_2/HC = 174), which was a very slow feedrate where accurate sample collection was difficult, the product mole percentages are either small or do not change significantly as the H_2/HC ratio decreases. Therefore, for the range of data investigated with the lowest ratio corresponding to the maximum feedrate obtained without plugging the lines of the system, it may be assumed that a large "pool" of excess hydrogen is available and

TABLE 4.13

Feedstock Conversion as a Function of % Fluorene in Decalin

% Fluorene in Decalin Feedstock	% Conversion		
	fluorene	trans-decalin	cis-decalin
0.1	0.0	58.9	97.1
5.1	94.9	27.5	92.9
9.5	84.7	-6.0	74.0
14.6	64.7	-15.1	46.5
19.4	63.4	7.7	86.3

TABLE 4.14

Concentration of Compound Groups as a Function of H_2/Hydrocarbon Ratio.

H_2/HC	Compound Group Product Conc./kg-mole/m^3 x 10^5												
	ALK	CPT	CHX	BZ	DMOHP	TD	CD	TT	IN	NAP	BIP	FL	MFL
173.8	97.6	19.8	3.4	26.7	9.4	24.5	2.7	1.8	16.0	9.3	3.9	4.1	1.7
84.9	131.4	34.1	7.9	54.2	20.6	62.5	8.2	3.7	31.0	25.3	11.9	9.5	3.9
41.8	115.3	45.2	10.5	102.1	50.7	186.7	42.8	6.0	44.6	30.7	19.0	28.2	11.4
26.0	238.3	62.1	13.6	171.4	87.9	349.4	113.7	9.9	65.9	44.4	30.0	73.4	21.6
21.1	150.5	51.9	11.8	160.0	87.7	454.7	208.9	11.7	62.0	44.8	54.2	122.2	19.5

TABLE 4.15

Conversion of Feedstocks as a Function of H_2/HC Ratio.

H_2/HC	% Conversion		
	fluorene	trans-decalin	cis-decalin
173.8	86.4	50.3	96.4
84.9	84.3	36.6	94.5
41.8	63.4	7.7	86.3
26.0	57.0	-13.1	76.9
21.1	42.8	-17.7	66.1

TABLE 4.16

Feedstock Free Mole % Product Dstribution of H_2/HC
Experimental Series

H_2/HC	Compound Group Product Dist., Mole %								
	ALK	CPT	CHX	BZ	DMOHP	IN	NAP	BIP	NFL
173.8	50.8	10.3	1.8	13.9	7.2	8.3	4.8	2.0	0.9
84.9	41.0	10.7	2.5	16.9	6.4	9.7	7.9	3.7	1.2
41.8	26.4	10.0	2.3	24.1	12.2	10.6	7.1	4.6	2.7
26.0	32.4	8.5	1.8	23.3	12.0	9.0	6.0	4.1	2.9
21.1	23.4	8.1	1.8	24.9	13.7	9.6	7.0	8.4	3.0

the only effect found is an increase in concentration for each group with increasing feedrate.

Conversion, on the other hand, decreases for each feedstock with decreasing hydrogen/hydrocarbon ratio where trans-decalin is eventually produced instead of consumed. This drop in conversion is outweighed by the increase in fluorene/decalin feedrate hence concentrations show an increase as more hydrocarbons are present at reactor conditions.

For these runs, the independent variable of the kinetic model, space-time, remained constant due to the large excess of hydrogen present. It has been shown, however, that the effect of hydrogen to hydrocarbon ratio is fairly linear for the concentrations of the compound groups and should not change the overall kinetic model or the relative magnitudes of the rate constants even though their absolute values would change if the feedrate was changed from that of the space-time and temperature experiments. Therefore, the results of these feed ratio experiments do place a constraint on the flexibility of the kinetic model. This constraint may be relaxed somewhat by the fact that over the range of experimentation, hydrogen is in excess and that its primary contrbution is to keep the active sites "clean" by controlling coke formation as was discussed for run 59 where helium was used as a carrier gas and coking was severe.

5) Catalyst Activity and Coking

From both a practical standpoint and for correct analysis of the kinetics of the fluorene/decalin system, the activity and extent of

coking of the zeolite catalyst should be established. A loss of catalyst activity is due to three primary causes (Froment and Bischoff, 1979):

1. Structural changes in the catalyst itself, such as sintering or migration of the metal on the catalyst.
2. Poisoning, the irreversible chemisorption of some impurity in the feed stream.
3. Deposition of carbonaceous residues from reactant, intermediate or product of the reaction, which is termed coking.

These effects on catalyst activity were investigated by several studies. The effect of pressure was determined by varying the hydrogen pressure from 8.2 to 35.8 bar while maintaining other conditions constant. The variation of pressure can also eludicate reaction mechanisms if changes are found to occur in the product distrbution. Because of the complex nature of the reactions investigated in this study, one cannot hope to pinpoint specific reaction mechanisms, such as dual or single site. Rather, one might hope that the response of the various products to a change in pressure would at least indicate that several products are formed by somewhat the same or different mechanisms.

Deactivation was observed at 633 and 661°K in relatively long run times of 6.5×10^4 s compared to the typical base run time of 1.2×10^4 s. The catalyst was regenerated and the weight and weight percent of coke on the catalyst, were recorded for runs 72 to 124 to investigate the effects of the variables in the study on coke formation.

The catalyst was also tested without nickel in run 116, thereby removing the sites thought to promote the hydrogenation/dehydrogenation

function. No reaction was observed, therefore the nickel sites are required for the reaction to be initiated. As discussed earlier, helium was used in run 59 as the carrier gas where it was found that coking was severe.

i) Effect of Pressure

The effect of pressure on the product distribution is best observed by comparing the feedstock free mole percentages of the products due to changes in concentration with pressure in the reactor. A summary of the pressure series runs is shown in Table 4.17 were all conditions are constant except for the total pressure at the reactor. The results of this work are shown in Table 4.18 as feedstock free product distribution and conversion of the feedstocks. No significant change in conversion is shown for the range of pressures investigated for the operating conditions of the reactor system (8.2 to 35.8 bar). Fluorene and cis-decalin conversions are relatively constant and trans-decalin conversion is first positive and then negative indicating an equilibrium reaction being obtained with cis-decalin.

The product distribution does change with respect to three compound groups. As pressure increases, DMOHP increases and naphthalenes decrease in mole percent with no significant changes noted in the other products. This is an indication of a shift in the decalin reaction from one of dehydrogenation to naphthalenes toward isomerization forming DMOHP and trans-decalin. The fraction of indanes also decreases somewhat with increasing pressure indicating that it is also tied into the decalin dehydrogenation/isomerization reaction. This insight into the reaction scheme is the primary result of the pressure work because the effect of pressure is small on the product distribution and not

TABLE 4.17

Summary of Pressure Series Run Conditions.

Operating conditions:

Catalyst: 5% Ni on LZ-Y62 zeolite; 20/40 mesh.

Feedstock: 20 wt % fluorene in decalin isomers

Feedrate: 2.84×10^{-9} m^3/s

Temperature: 661°K

H_2/HC ratio: 41.8 kg-mole/kg-mole

H_2 feedrate: 7.05×10^{-7} kg-mole/s

Run[a]	Press./ bar	Molar Gas Density/kg-mole/m^3	Cat Vol/ $m^3 \times 10^6$	Cat Wt/ kg $\times 10^3$	Space-time/s
124	8.2	0.149	24.5	13.61	5.1
BASE	14.8	0.269	13.0	7.005	4.8
123	25.1	0.458	7.7	4.129	4.9
122	35.8	0.653	5.5	3.036	4.9

a: Detailed run conditions may be found in Appendix 3.

TABLE 4.18

Feedstock Free Product Distribution and Feedstock Conversion of Pressure Series.

	Feedstock Free Compound Group Product Distribution, Mole %								
P/bar	ALK	CPT	CHX	BZ	DMOHP	IN	NAP	BIP	MFL
8.2	29.7	7.3	1.6	19.4	9.9	15.4	9.8	4.2	2.7
14.8	26.4	10.0	2.3	24.1	12.2	10.6	7.1	4.6	2.7
25.1	25.1	10.0	2.7	24.9	15.0	9.9	5.9	4.2	2.4
35.8	22.3	8.2	2.0	25.5	20.4	8.8	5.4	4.9	2.5

	% Feedstock Conversion		
P/bar	fluorene	trans-decalin	cis-decalin
8.2	68.5	6.3	89.1
14.8	63.4	7.7	86.3
25.1	63.6	-3.8	86.6
35.8	53.6	-11.6	81.1

significant where conversion is concerned, for the range of pressure investigated.

ii) Catalyst Deactivation

Deactivation is of importance because it determines in many cases the need for regeneration, or controls the useful life of the catalyst. Since the feedstock used did not contain poisons to the catalyst and regeneraton restored activity, then it may be assumed that the decrease in activity with run time is due to coking of the catalyst (Froment and Bishoff, 1979). Therefore deactivation experiments should indicate the nature of the coking by observing the changes in the distribution of the product compound groups with run time. From Levenspiel (1972), the rate of deactivation of a catalyst pellet may be written as:

$$\text{Deact. rate} = f_1\ (\text{Temp.}) \cdot f_2(\text{Conc.}) \cdot f_3\ (\text{Cat. Condition}) \qquad 4.5$$

which is similar to the reacting species equation with the addition of a deactivation function.

Deactivation was investigated in run 91 (661°K) with seven material balances and in run 117 (633°K) with five balances made as each run progressed. These run conditions are summarized in Table 4.19. When deactivation is due to coking, if the selectivity is altered, the nature of the kinetic model may be further complicated by the addition of deactivation terms depending on which concentrations are involved. However, if coking is uniform, and selectivity does not change appreciably, then the reaction only suffers from an overall deactivation. As shown in Figures 4.9 and 4.10, conversion of the feedstocks does indeed drop except for trans-decalin which is formed in the 633°K runs and essentially unreactive in the 661°K series. This drop in conversion with run time indicates deactivation due to the effects of coking.

TABLE 4.19

Summary of Deactivation Run Conditions at 633 and 661°K.

Operating Conditions:

Catalyst: 5% Ni on LZ-Y62 zeolite, 20/40 mesh.

weight = 7.016×10^{-3} kg

volume = 1.3×10^{-5} m^3

Feedstock: 20 wt % fluorene in decalin isomers

Feedrate: 2.84×10^{-9} m^3/s

H_2/HC ratio: 41.5 kg-mole/kg-mole

H_2 feedrate:

7.14×10^{-7} kg-mole/s for 661°K run.

7.02×10^{-7} kg-mole/s for 633°K run.

Space-time/s: 4.8 for 661°K run

5.2 for 633°K run

Pressure: 14.8 bar

633°K Run 117[a] Material Bal No.	Run Time/s[b]	661°K Run 91[a] Material Bal No.	Run Time/s[b]
1	13680	1[c]	9110
2	26110	2	16590
3	39960	3	24400
4	54760	4	31950
5	64240	5	39910
		6	50730
		7	62380

a: Detailed Run Data may be found in Appendix 3.

b: Average time between start and end of material balance.

c: C bal closure = 84 %, not included in analysis.

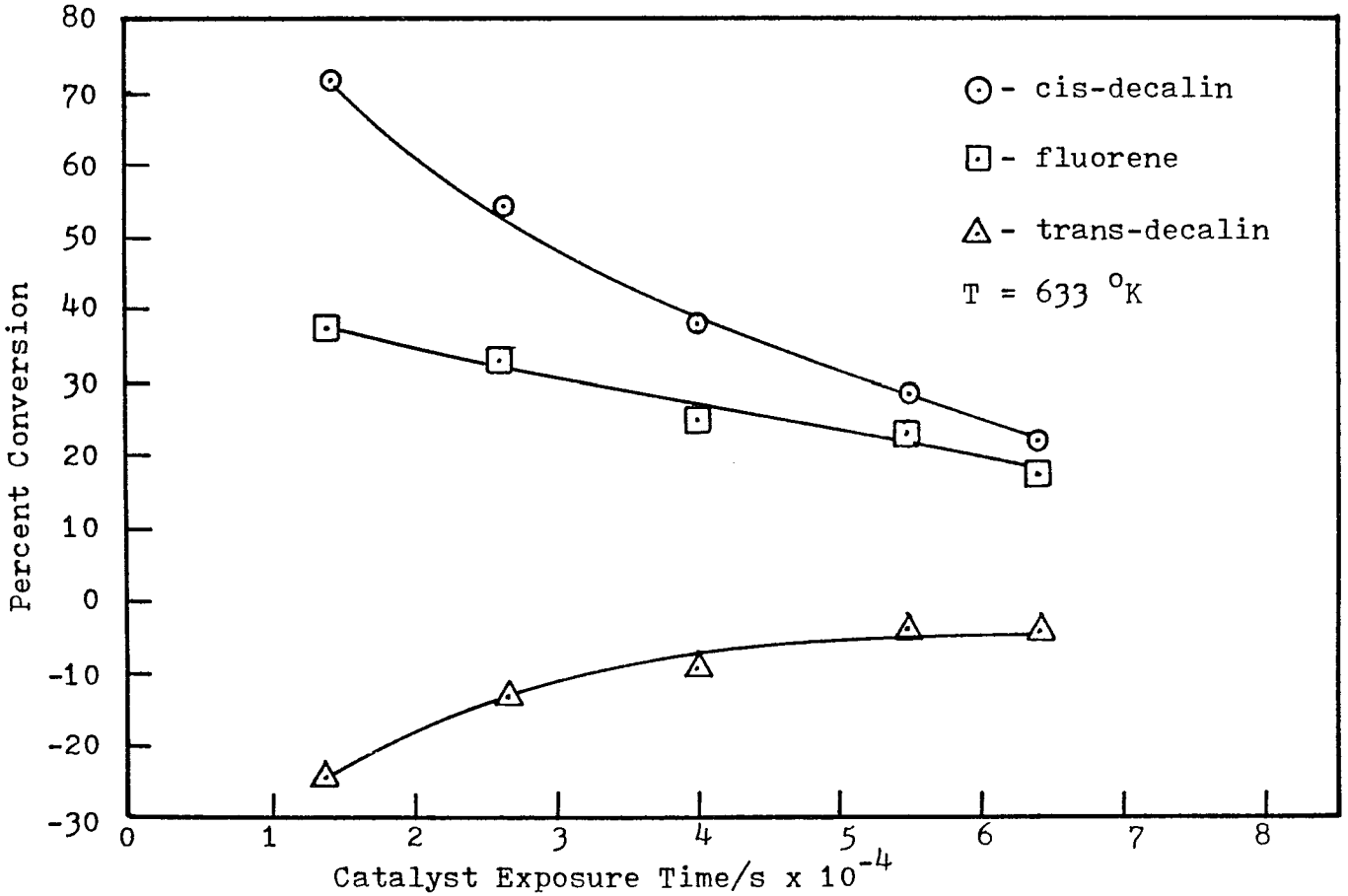


FIGURE 4.9 Conversion of Feedstock Components as a Function of Run Time

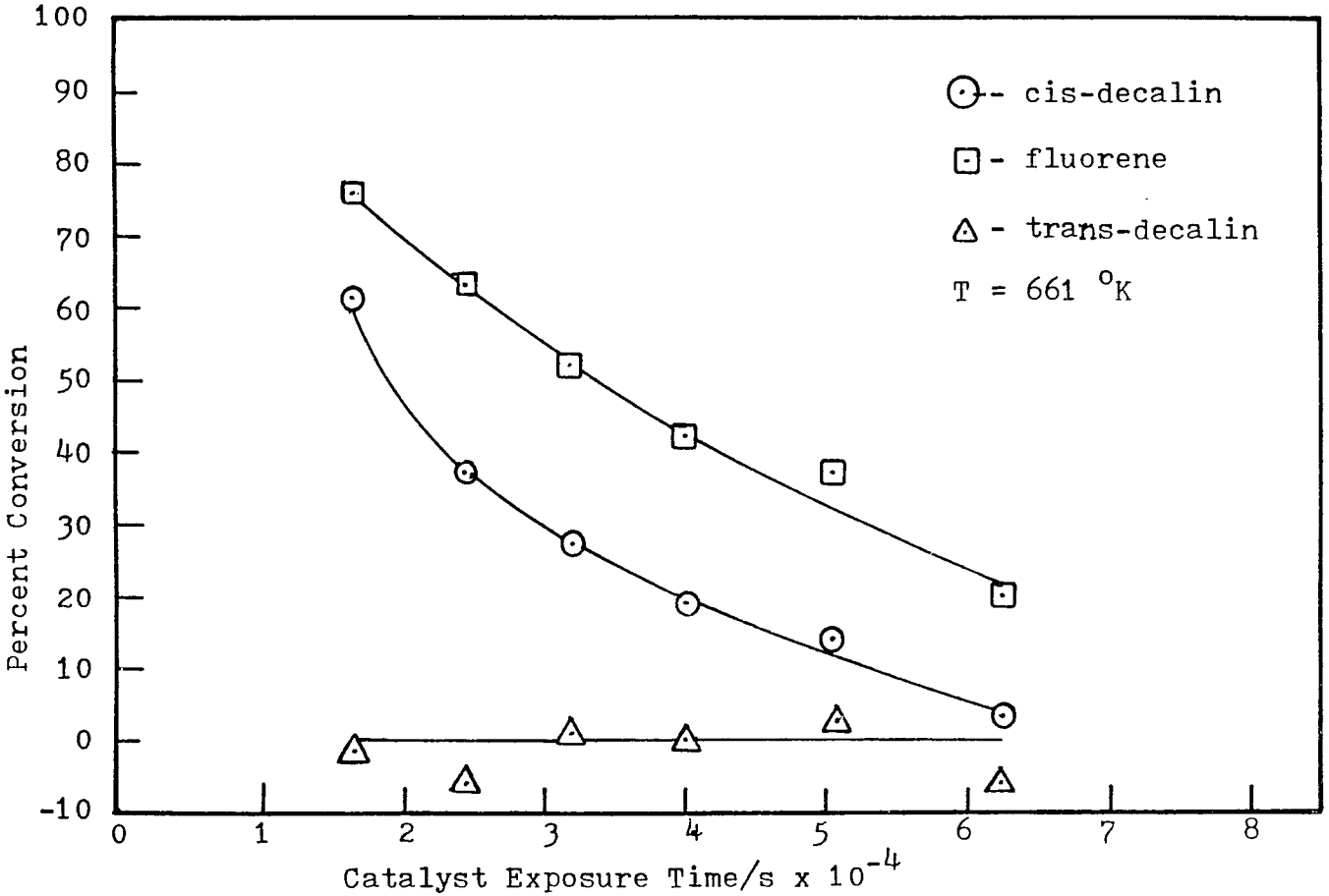


FIGURE 4.10 Conversion of Feedstock Components as a Function of Run Time

However, as shown in Table 4.20, at both temperatures the feedstock free product distribution does not change significantly with catalyst exposure time. Therefore, selectivity is maintained.

In light of this observation, and considering the complex model developed in the next chapter to describe the kinetics based on space-time and temperature data, the effect of deactivation is not included. This is a simplifying assumption, but it was not felt that the addition of a deactivation rate would add clarity to the model as the source of the coke formation could not be determined. Deactivation does not affect the results of this study as all experiments were performed with approximately the same catalyst exposure time of 1.2×10^4 seconds. Therefore, the quantitative effects of deactivation on the kinetic model must be left unanswered at present.

iii) Coking and Regeneration

The catalyst prepared for the runs in the experimental series was divided into eight equal quantities and used in a random order with regeneration after use providing a determination of the coke accumulated, as weight of coke and weight % coke of the dry catalyst. This random order of catalyst use, for which a history was recorded, was done to avoid bias in the data if the same catalyst was used repeatedly. The experiments were also not performed in series for the same reason. Activity of the catalyst remained the same as was shown by the base run comparison. Run 93 catalyst had been regenerated five times, run 94 catalyst four times, run 95 once, and run 114 catalyst four times without biased results.

The results of the coke analyses are presented in Table 4.21 as weight % coke on the catalyst to normalize the runs where catalyst weight

TABLE 4.20

Feedstock Free Product Distributions of Deactivation Runs at 661 and 633°K.

	Feedstock Free Product Dist., Mole %, 633°K								
Run Time/s	ALK	CPT	CHX	BZ	DMOHP	IN	NAP	BIP	NFL
13680	23.2	2.2	0.8	23.1	11.7	14.5	10.0	9.4	4.9
26110	16.3	6.8	1.8	26.8	18.0	9.6	7.4	9.2	4.1
39960	19.0	1.6	0.8	25.6	17.1	9.8	8.9	12.3	4.8
54760	22.0	2.2	1.0	23.3	15.7	6.1	10.4	14.3	5.0
64240	20.3	7.2	1.8	23.7	13.6	5.6	9.2	13.2	5.3

	Mole % Dist., 661°K								
Run Time/s	ALK	CPT	CHX	BZ	DMOHP	IN	NAP	BIP	NFL
9110	50.8	4.3	1.3	19.3	7.2	8.4	5.7	2.1	0.9
16590	47.9	6.8	1.4	19.3	7.6	7.2	5.3	2.7	1.8
24400	51.1	8.3	1.4	14.2	6.3	4.1	6.3	5.7	2.6
31950	36.2	13.2	1.9	18.1	5.4	6.6	8.1	7.0	3.3
39910	40.9	9.5	1.5	16.7	5.3	6.7	7.1	8.1	4.1
50730	48.7	6.0	1.1	14.8	2.8	8.2	7.4	7.8	3.3
62380	50.5	3.3	1.8	13.1	2.9	9.5	7.2	8.2	3.4

TABLE 4.21

Effect of Experimental Variables on Wt. % Coke of Catalyst Weight.

T/°K	% coke
632.8	12.11
639.5	10.72
649.8	16.47
655.4	11.46
661.0	10.25
667.0	13.80
672.6	7.89
677.7	12.53
683.5	11.29
688.2	19.84

% fluorene in feedstock	% coke
0	12.53
20	10.25

H_2/HC	% coke
173.8	3.66
84.9	7.61
41.8	10.25
26.0	13.42
21.1	7.18

P/bar	% coke
8.2	7.51
14.8	10.25
25.1	11.10
35.8	10.30

% Ni on Catalyst	% coke
0	1.89
5	10.25

Space-time/s at 633°K	% coke
0.45	15.90
0.75	17.81
0.93	15.14
1.6	16.37
3.1	15.15
5.1	9.58

Space-time/s at 661°K	% coke
0.36	21.54
0.92	21.56
1.6	18.99
2.4	19.82
4.8	10.25

TABLE 4.21 (continued)

Gas Velocity/m/s	% coke
7.1×10^{-3}	10.79
13.8×10^{-3}	10.25
20.1×10^{-3}	10.93

Particle Size/633°K	% coke
20/40 mesh	9.58
60/80 mesh	6.46

Particle Size/661°K	% coke
20/40 mesh	10.25
60/80 mesh	7.23

Run Time/s @ 661°K	% coke
1.292×10^{4}	10.25
2.903×10^{4}	15.83
6.424×10^{4}	17.74

Run Time/s @ 633°K	% coke
1.289×10^{4}	9.58
6.617×10^{4}	13.11

was different. No trends are indicated in % coke with temperature, pressure, or fluorene/decalin ratio and except for a sudden drop in % coke at the longest space-time for either temperature, no effect is found. A fairly constant weight percent of coke over the range of temperature, pressure, and liquid feed ratios was not expected but does show that the amount of coke formed is not a function of these variables over the range investigated. Decalin makes a significant contribution to coke and possibly masks any coke from fluorene as the percentage did not change with the liquid feed ratio.

Now, looking at the coke from the hydrogen/hydrocarbon ratio runs, it increases on the catalyst with decreasing feedstock ratio confirming the previous feedstock ratio observation that hydrogen in the gas has the primary role of controlling the coke and keeping the catalyst relatively clean. The coke found on the catalyst is low in the H_2/HC = 21.1 run because the run time was short due to operating difficulties at this high liquid feedrate.

In run 116, the catalyst was used without nickel and coke formation was negligible with no reaction observed. Once again, the metal sites are required for the reaction to be initiated.

In relation to the transport studies, changing gas velocity had no effect but reduction in particle size did decrease coke formation. This indicates that some diffusional limitations may exist but this change in coke is not as significant as the pore diffusion limitation study as the nature of coke formation was not thoroughly established in this study. The catalyst in both 60/80 mesh runs was used late in the study and had been regenerated several times. Some coke always remains on the catalyst after regeneration which would decrease the measured amount in

these late runs by occupying coke sites before the reaction started. Therefore the results of coking with changing particle size are uncertain and the transport results are still valid.

A definite trend is indicated with run time and this weight percent data was treated at 661°K by using the empirical Voorhies (1945) correlation:

$$C_c = a\ \tau^n \qquad 4.6$$

where:

C_c = weight percent coke on catalyst.

a = f(feedstock, catalyst, temperature)

n = constant.

τ = run time/s (catalyst exposure time).

By least squares analysis of a power fit, the resulting correlation is:

$$C_c = 0.42 \quad (\tau)^{0.34} \qquad 4.7$$

The result of this fit is shown in Figure 4.11. With this correlation, an estimate of the coke with run time for the base conditions can be made to estimate when to regenerate the catalyst.

Although an expression has been developed for the amount of coke built up with run time, coke was not included in the material balance calculations or the kinetic model. The effect of coke formation was found not be as significant as one would expect in the material balance. The amount of coke formed was estimated, assuming the coke was pure carbon, using the Voorhies correlation for the time period of the material balance. Comparison of material balance results are shown in Table 4.22 using run 114 as an example, with and without coke in the products. The material balance closure was not significantly changed and the product concentration distribution is approximately the same.

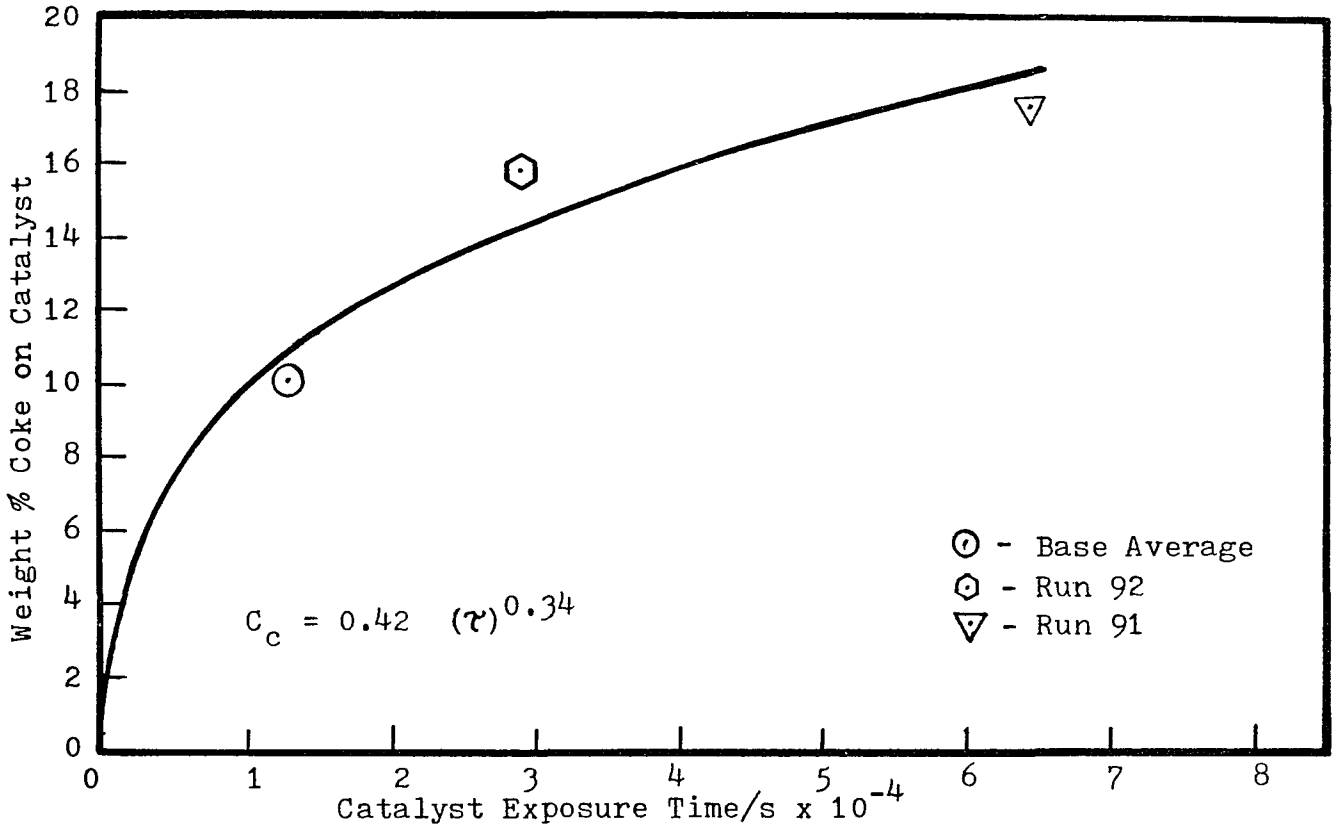


FIGURE 4.11 Weight Percent of Coke on Ni/LZ-Y62 Catalyst by Voorhies (1945) correlation at 661°K and 14.8 bar.

TABLE 4.22

Material Balance Results of Run 114 with and without Coke.

Compound Group	Concentration/kg-mole/m^3 x 10^5 Without Coke	With Coke
ALK	125.1	124.7
CPT	53.4	53.2
CHX	12.6	12.6
BZ	104.9	104.5
DMOHP	55.9	55.7
TD	193.4	192.7
CD	33.7	33.6
TT	6.5	6.4
IN	50.2	50.0
NAP	30.9	30.8
BIP	18.0	17.9
FL	42.4	42.2
MFL	12.5	12.5
Coke	0.0	87.7

To test the assumptions, coke was included in the kinetic model for space-time assuming that it was formed by several different routes. None of these routes improved the fit of the model to the experimental data. Therefore, since the source of the coke could not be determined and its exact composition was unknown, this reaction was not included in the kinetic model or material balance calculations.

6) Literature Cited

Bryant, P.A., "Hydroisomerization of Normal Pentane over a Zeolite Catalyst", Ph.D. Dissertation, L.S.U. (1966).

Froment, G.F. and K.B. Bischoff, Chemical Reactor Analysis and Design, J. Wiley, New York (1979).

Hill, C.G., An Introduction to Chemical Engineering Kinetics and Reactor Design, J. Wiley, New York (1977).

Levenspiel, O., Chemical Reaction Engineering, 2nd ed., J. Wiley, New York (1972).

Satterfield, C.N., Heterogeneous Catalysis in Practice, McGraw-Hill, New York (1980).

Voorhies, A., Ind. Eng. Chem., 37(4), 318 (1945).

CHAPTER V

Application of Results to the Kinetic Model

1) Introduction

The purpose of this chapter is to apply the experimental results discussed in Chapter IV to formulate a kinetic model and propose a reaction mechanism. In order to do this, the experimental results must be summarized and then various models tested with the concentration vs. space-time data to arrive at an acceptable model for the reaction scheme.

The method of Himmelblau et al. (1967) was used to approximate the kinetic equations with two methods employed to solve the resulting matrices. For a direct solution, Gauss-Jordan elimination was used as presented by Carnahan et al. (1969) and converted to BASIC from FORTRAN for this study. This direct approach was found inadequate, however, as it tended to generate negative rate constants in many of the models tested. Therefore, a pattern search routine (Moore et al., 1969) was applied with constraints to generate all positive rate coefficients. With all positive rate constants obtained, the LSODE routine (Hindmarsh, 1980) was used to numerically solve the differential equations of the model. The predicted concentrations of the compound groups were then compared to the experimental data to determine if the model equations predicted the effect of space-time on concentration.

Once the rate coefficients were obtained, the activation energy for each reaction path was estimated from the concentration vs. temperature data using the 661°K space-time data as a base. A reaction mechanism was then proposed, based on the results of each experimental series and

the complex reaction pathways of the final kinetic model. The following sections discuss each of these points in detail and present the kinetics of the reaction of fluorene in decalin on a zeolite catalyst.

2) Observations from Experimental Results

i) Limitations Observed

There were no thermal reactions observed in this study as evidenced in run 28 from 478 to 789°K. No significant transport limitations were found for either external mass transfer or pore diffusion for the range of temperatures used in formulating the kinetic model (633 to 661°K). However, configurational diffusion limitations may cause reaction at the external surface of the particles.

Hydrogen pressure was not found to have a significant effect on the reaction except for a shift in the cis-decalin reaction from one of dehydrogenation to isomerization and cracking. This effect was small relative to the effect of temperature and space-time on concentration and although the pressure experiments resulted in part of decalin reaction scheme being defined, pressure effects were not significant for the kinetic model.

The effects of deactivation of the catalyst with run time were not included in the kinetic model due to the complex nature of both the model without deactivation terms and the uncertainty of the route of coke formation contributing to deactivation. As was shown in Chapter IV, accounting for coke had little effect on the concentration terms from the material balance. Regeneration of the catalyst back to a high activity removed coke and did not affect the runs where catalyst was used repeatedly. The nature of coke formation and inclusion of a

deactivation rate into the proposed model should be considered as a point to recommend for future study as its formation with run time for base conditions has been determined by the Voorhies correlation. Adding the dimension of run time to the kinetic model would be a starting point for this analysis. For the present, the effect of coke formation and the resulting deactivation of the catalyst is a limitation of the kinetic model developed.

An effect of feed ratios (fluorene/decalin and hydrogen/hydrocarbon) was noted but selectivity was not significantly affected and several important observations were made providing insight into the reaction scheme. These will be discussed with other reaction scheme observations in the next section. In all space-time and temperature studies, feed ratios were held constant.

ii) Role of Decalin, Catalyst, and Hydrogen

Insight into the reaction scheme was provided by each experimental series and the first group of qualitative runs. Each component (donor solvent, catalyst, and molecular hydrogen) was found to play an important role in the conversion of fluorene to gasoline fractions.

a.) Decalin Contribution

A hydrogen rich solvent of fairly high boiling point was found essential for the fluorene reaction to proceed. Tetralin is commonly used as a donor solvent (EDS process); however, it was found in the tetralin experiments that in comparison, decalin was a more suitable solvent as it produces more benzenes and less naphthalenes than tetralin. Tetralin formed more complex benzenes and the large fraction

of naphthalene produced would require hydrogenation for recycle as a donor solvent.

The two isomers of decalin found in the practical grade mixture both contribute to the reaction and reactor system operation. Cis-decalin was found reactive and is assumed to contribute to the hydrogenation of fluorene. On the other hand, trans-decalin was fairly unreactive but contributes to the operation of the product recovery section of the reactor system as it serves as a solvent for heavier components and fluorene in the product mixture. It was only necessary to dissolve the product samples in dichloromethane for runs where fluorene crystallized at room temperature after cooling from the heated primary condenser.

Three primary routes for transformation of decalin were found, viz. the dehydrogenation of cis-decalin to tetralin, promoting the hydrogenation of fluorene, isomerization occurring in a reversible reaction with trans-decalin and DMOHP, and the direct cracking of cis-decalin to cyclohexanes and alkanes (gas).

b.) Catalyst Contribution

The specifics of the reaction mechanism involved on the catalyst surface could not be determined due to the complex kinetics involved with many compounds to account for; however, observations of this study allow the basic mechanism to be proposed, based on the theory and previous studies discussed in chapter II. An acidic Y zeolite was found necessary for the fluorene reaction as the Ru-Y zeolite tested, which was not acidic, did not cause fluorene to react. The Ru-Y type provided only for the dehydrogenation of decalin at the metal sites. The Ni-Y

zeolite used for the quantitative work was highly active and promoted both cracking and hydrogenation/dehydrogenation.

The proposed contribution from the catalyst is first to initiate the reaction by adsorption of fluorene into a reactive state. This is followed with a gas phase attack by decalin in a hydrogen transfer step similar to that of the Eley-Rideal (1941) mechanism discussed in chapter II. With fluorene partially hydrogenated, cracking occurs by the accepted carbonium ion mechanism, hence the contribution of the acidic sites is established. These acidic sites also crack decalin to lighter cyclics and alkanes and are responsible for any isomerization occurring. Any dehydrogenation is provided on the metal sites. However, the separation of these two sites, acidic and metal, is not as exact as it appears, since it was observed by Brignac (1984), using the same catalyst as in this study, that the presence of nickel promoted the effect of the acid function in the study of toluene disproportionation. The products of the fluorene/decalin reaction of this study were indeed highly substituted with methyl groups indicating that the same disproportionation reaction is occurring throughout the reaction scheme. As was discussed in Chapter II, Hall (1967) and other investigators have proposed that this increase in acidity of the catalyst is due to the reduction of the metal cation by hydrogen. This reduction was assumed to occur while hydrogen was flowing through the reactor overnight at a temperature of 700°K before each experimental run was started.

It is therefore proposed that the hydrogenation of fluorene adsorbed on the catalyst, from decalin in the gas phase, occurs before further fluorene reaction takes place on the catalyst sites. This was confirmed when no fluorene reaction occurred when aromatic solvents were

present. The requirement of first dehydrogenating decalin to tetralin was shown in run 116 where no reaction was observed without nickel on the catalyst.

c.) Hydrogen Contribution

It was found that a large "pool" of hydrogen was available to the reaction and without it, coking was severe and no reaction occurred. Based on the experimental results, hydrogen is required but acts essentially to keep the catalyst "clean" for reaction of decalin and fluorene. Material balance results show that in the majority of runs, molecular hydrogen was not consumed, but produced. Overall, the change in hydrogen flowrate was minor from inlet to exit, therefore the assumption is made that molecular hydrogen primarily controls coke formation and is available in excess for the hydrocarbon reactants. As noted above, hydrogen is also essential to reduce the metal on the catalyst.

iii) Summary of Reaction Path Observations

Before beginning work on the kinetic model, a careful study of the experimental results was made as discussed in chapter IV to postulate how each product was formed. These observations are summarized below as a starting point for the kinetic model.

1. Hydrogen gas serves to reduce coke formation on the catalyst so that hydrocarbons may react.
2. Initial products of fluorene are biphenyls, indanes, and benzenes.

3. DMOHP is an isomer of decalin which reacts to form cyclopentanes and alkanes.
4. Decalin has four routes: isomerization, dehydrogenation, cracking, and a gas phase attack, transferring hydrogen to fluorene adsorbed on the catalyst in a reactive state.
5. Alkanes appear to be formed primarily from decalin alone.
6. Coke formation is a function of time and was shown to be well correlated by the Voorhies equation. The coke "concentration" is not to be included in the model as its nature of formation could not be determined.
7. Deactivation, which is significant, is not included in the model as it was found to be a function of the coke formation which is not clearly understood.
8. The most significant effects on the reaction were space-time and temperature, hence they are the variables of interest.

3) Kinetic Model

i) Method and Development

The determination of rate coefficients is essential in any reaction study. With the model established, analysis, simulation, and design of reactor systems may begin. In heterogeneous catalysis, Langmuir-Hinshelwood-Hougen-Watson (LHHW) rate expressions are typically used to describe the kinetics as discussed by Froment and Bischoff (1979), Hill (1977), and many other investigators. This type of analysis accounts for both reaction and adsorption phenomena and is typically called LHHW kinetics after the analysis of adsorption by Langmuir (1916, 1918) and application to reaction mechanisms by Hougen and Watson (1943). This

type of analysis provides for accurate descriptions of the reaction mechanisms to be performed; however, for even simple reaction systems the number of terms involved and form of the expressions may be quite complex.

The reaction of decalin and fluorene on Ni-Y zeolites was found to be very complex with many products formed as shown in the experimental results. Grouping the compounds into parent structure groups simplified the data analysis somewhat; however, a complex reaction structure still remained. Therefore the following assumptions are made in addition to the summary of reaction path observations listed above.

1. The rate is primarily a function of space-time and temperature without pressure effects.
2. Pseudo-homogeneous rate expressions may be used to describe the kinetics as adsorption phenomena were not investigated.
3. Each compound group is treated as a single species where the reaction of each species is first order.

For these assumptions to be valid, the model must be shown to adequately fit the experimental data. This was done by employing the method of Himmelblau et al. (1967), further referred to as the HJB method, to determine the rate coefficients and then numerically solving the differential equations using the Hindmarsh (1980) routine, LSODE, as presented below.

First, the kinetic model is assumed to be composed to M independent equations of the form:

$$dC_1/dt=K_1R_{11}(t)+\ldots+K_kR_{1,k}+\ldots+K_NR_{1,N}(t)$$

$$\vdots$$

$$dC_j/dt = K_1 R_{j,1} + \ldots + K_k R_{j,k} + \ldots + K_N R_{j,N} \qquad 5.1$$

$$\vdots$$

$$dC_M/dt = K_1 R_{M,1} + \ldots + K_k R_{M,k} + \ldots + K_N R_{M,N}$$

and:

$$C_1(0) = C_{o,1}$$

$$\vdots$$

$$C_j(0) = C_{o,j}$$

$$\vdots$$

$$C_M(0) = C_{o,M}$$

where:

C_j = concentration of compound group j, kg-mole/m^3

t = space-time, s.

K = rate coefficient, in appropriate units for consistency with concentration term; if R is first order, K [=] s^{-1}.

R = concentration function with space-time.

Equation 5.1 may be abbreviated as:

$$dC_j/dt = \sum_{k=1}^{N} K_k R_{jk} \qquad (j=1,2,\ldots,M) \qquad 5.2$$

Solution of equation 5.2 may be made using the fact that the right hand side involves only integration of functions of measured concentration as functions of space-time. In other words, the integrated equations are linear in the coefficients and only integrals of the concentration terms are required.

Upon integration of equation 5.2 with respect to space-time from 0 to t_i one obtains the relation:

$$C_j(t_i) - C_j(0) = \sum_{k=1}^{N} K_k \int_0^{t_i} R_{jk}\,dt \qquad 5.3$$

$$(i=1,2,\ldots,P);(j=1,2,\ldots,M)$$

where P is the number of time intervals between measurement of concentrations. Equation 5.3 may be expressed as:

$$Y_{ij} = C_{ij} - C_{oj} = \sum_{k=1}^{N} K_k X_{ijk} \qquad 5.4$$

where X_{ijk} contains the integrated concentration terms and equation 5.4 represents a set linear in the coefficients, K_k, to be determined.

Since experimental data are to be used in calculating the "best" values of the K_k's, a satisfactory criterion must be employed. This is typically done by minimizing the sum of squares of the weighted deviations between the experimental and calculated values of Y_{ij} over all runs as:

$$F=\text{minimum} \sum_{\substack{\text{all}\\ \text{runs}}} \sum_{i=1}^{P} \sum_{j=1}^{M} [(Y_{ij}-\hat{Y}_{ij})W_{ij}]^2_{run} \qquad 5.5$$

where:

$Y_{i,j}$ = measured change in concentration

$\hat{Y}_{i,j}$ = predicted change in concentration

$W_{i,j}$ = $1/|Y_{ij}|$, weighting factor converting each absolute deviation to a relative deviation.

The expression F, to be minimized, is a quadratic function of the K_k's, and therefore represents a surface with only one extremum (a minimum) in N dimensional space. It is therefore possible to obtain a set of consistent simultaneous algebraic equations by equating all the first partial derivatives of F with respect to K_k equal to zero. This

set of equations has the unique solution **K** and yields a set of K_k's. Differentiating equation 5.5 and setting the result equal to zero yields:

$$\frac{\partial F}{\partial K_k} = 0 = \sum_{i=1}^{P} \sum_{j=1}^{M} [2W_{ij}^2 (Y_{ij} - \sum_{L=1}^{N} K_L X_{ijL})(-X_{ijk})] \qquad 5.6$$

or:

$$\sum_{L=1}^{N} \sum_{i=1}^{P} \sum_{j=1}^{M} (K_L W_{ij}^2 X_{ijk} X_{ijL}) =$$

$$\sum_{i=1}^{P} \sum_{j=1}^{M} (W_{ij}^2 Y_{ij} X_{ijk}) \qquad 5.7$$

$$(k=1,2,\ldots,N)$$

therefore in matrix notation:

$$\mathbf{S\ K = G} \qquad 5.8$$

where: $$s_{kL} = \sum_{i=1}^{P} \sum_{j=1}^{M} (W_{ij}^2 X_{ijk} X_{ijL})$$

$$(L=1,2,\ldots,N)$$

$$(k=1,2,\ldots,N)$$

and: $$g_k = \sum_{i=1}^{P} \sum_{j=1}^{M} (W_{ij}^2 Y_{ij} X_{ijk})$$

$$(k=1,2,\ldots,N)$$

with the solution vector:

$$K = \begin{bmatrix} K_1 \\ K_2 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ K_N \end{bmatrix}$$

The solution of equation 5.8 is then:

$$\mathbf{K = S^{-1}\ G} \qquad 5.9$$

which was determined by a Gauss-Jordan routine from Carnahan et al. (1969) converted from FORTRAN to BASIC.

This summarizes the technique of the HJB method to determine rate coefficients as a direct solution from a set of simultaneous equations linear in K_k. A part of this routine which is necessary for solution is the integration of the concentration term expressions, R_{ijk}. This numerical integration may be performed by the trapezoid rule to evaluate:

$$X_{ijk} = \int_0^{t_i} R_{jk} dt \qquad 5.10$$

noting that this integral starts at t=0 and is evaluated to t_i for each Y_{ij} to be determined from equation 5.4. The R_{jk} term then must be input to the numerical integration routine for each space-time for which that concentration was obtained, therefore, this generates the R_{ijk} terms of the matrix where the subscripts are:

i=space-time interval

j=compound group number

k=reaction path number, rate coefficient of reaction k.

The trapezoid rule employed, which may be expressed for example at a space-time equal to three seconds, i=3, with a step of one second, for compound group j and rate coefficient k as:

$$X_{3,j,k} \tilde{\sim} (1) \left[\frac{1}{2} R_{ojk} + R_{1jk} + R_{2jk} + \frac{1}{2} R_{3jk} \right] \qquad 5.11$$

requires that the time steps be equal, and this was not the case for the experimental concentration vs. space-time data. To obtain concentration data at equal time intervals, the experimental concentrations were plotted vs space-time and the concentration at equal time intervals was determined where a straight line crossed the interval of interest

between the experimental data. An example of this technique is shown in Figure 5.1 for one compound group of the 661°K space-time series. It should be noted that this is not a smoothing operation except in cases where data scatter was significant. The method of using straight lines between data points is necessary to avoid altering the material balance closure, which may occur if a smooth curve is drawn through the data points.

Once the rate coefficients were determined, the predicted concentrations from the LSODE routine were compared to the experimental data to decide if the model fitted the data. This is a more representative test of the model against the experimental data than to compare it to the adjusted concentration values. The program for this solution method may be found in Appendix 4 under the heading HJB.KINETIC.FIT. Implementation requires initial concentration data, the adjusted concentrations vs. space-time intervals and a list of R_{ikj} terms that are equated to the concentration terms describing the kinetic model of interest.

The method of attack to obtain rate coefficients was as follows. Based on the observations of the experimental results, reaction schemes were drawn and from them, the rate equations of the form of equation 5.1 were written. This generated the matrix of R_{ikj} terms which are listed in HJB.KINETIC.FIT that calls the data set, KINDAT730-2, of concentration vs. space-time data at a given temperature (661°K) which is also listed in Appendix 4. This routine was run on an Apple IIe personal computer from which rate coefficients were determined and substituted back into the kinetic model equations.

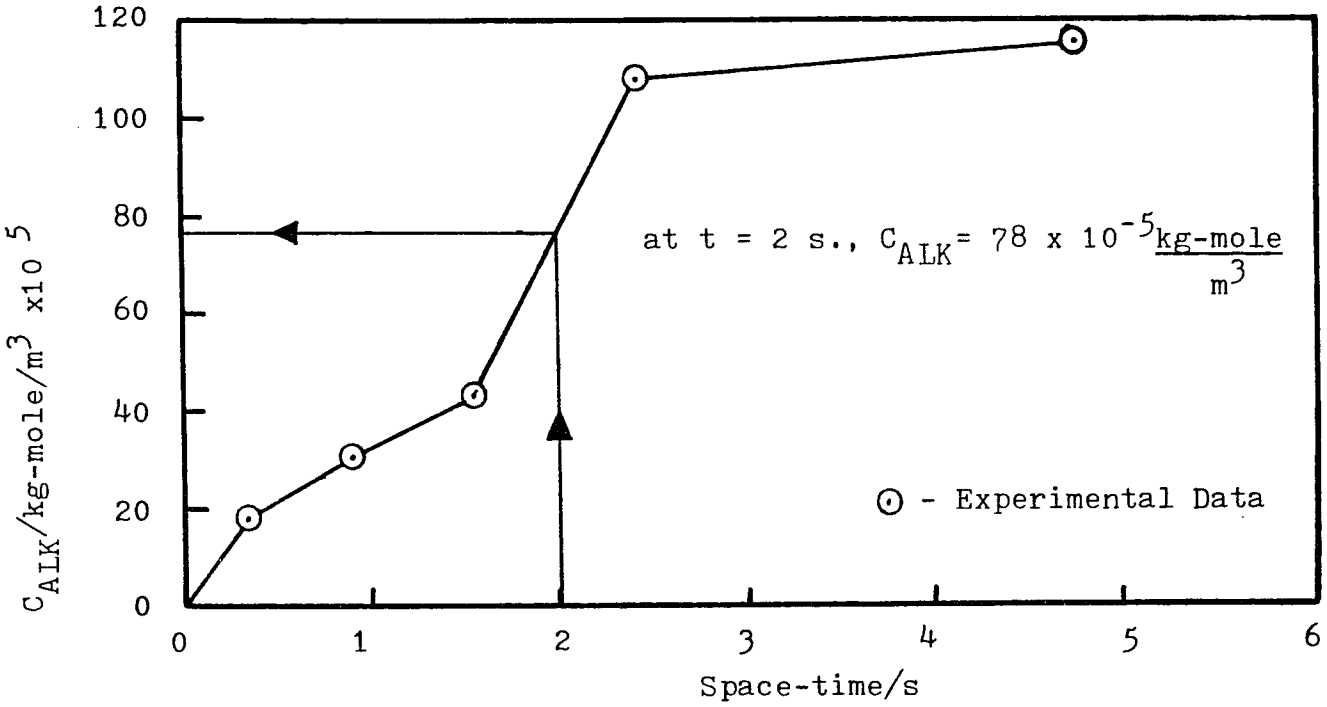


FIGURE 5.1 Example of Graphical Technique to Adjust Concentration to Equal Space-time Intervals. (Alkanes shown for 661°K space-time series)

The differential equations were then solved by the KINT730 routine listed in Appendix 4 which calls the LSODE routine from direct access disk on the IBM 3081 mainframe at Louisiana State University. LSODE uses the Gear-Hindmarsh integration method (Hindmarsh, 1980) efficiently solving the differential equations and listing the predicted concentrations for each compound group with space-time. The predicted concentrations were plotted and compared to the experimental data to estimate the validity of the model of interest. If the model did not describe the trends of the experimental data, the model was revised, new equations were written, and the HJB.KINETIC.FIT routine was used to estimate new rate coefficients. The new model was then checked by solution from LSODE (KINT730) with experimental data. This procedure was repeated until an adequate model was obtained.

A problem was encountered inherent in the minimization of the sum of squares of the weighted deviations in the Gauss-Jordan routine. In this calculation, for many models tested, several of the resulting rate coefficients would be negative and this result could not be used to evaluate the kinetic model. However, after many trials, a basic model was obtained by the direct solution technique of HJB.KINETIC.FIT yielding all positive rate coefficients. Evaluation of many models could not be done by this method because of the generation of negative rate coefficients so a more efficient analysis technique was developed so that every model proposed could be run in LSODE to evaluate the predicted vs. experimental results.

Using the criterion of equation 5.5, the rate coefficients were determined by a pattern search routine that was available from the Chemical Engineering Department. This routine is based on the pattern

search program of Moore et al. (1969), with modifications from this study to include the numerical integration routine. By this technique, which allows for constraints to be made on the solution, the rate constants were constrained to always be positive. Solution could then be made for each model provided optimization was obtained in the pattern search. Overall, this was found to be a more efficient technique than the Gauss-Jordan routine where only after many attempts could a model be tested in LSODE.

The program containing the pattern search routine is listed under the heading FIT730 in Appendix 4. The main program requires initial guesses of the rate coefficients and an initial step size and the number of step size reductions to perform at each optimization attained. Subroutine PATERN is the search routine which was not changed from the program of Moore et al. (1969). Subroutine BOUNDS constrains all rate coefficients to be positive, and Subroutine PROC contains the list of terms for evaluation of the kinetic model, the numerical integration, and the function to be optimized, which is the weighted sum of squares of the deviations.

Execution times for pattern search routines tend to be long, therefore the execution was halted so that initial guesses and step sizes could be improved and then the routine was rerun. This greatly reduced the execution times required for optimization.

In attempting to make a sound statistical analysis, a problem arises. Since the dependent variables (concentration) are taken over a successive series of space-time variables, they are not statistically independent as required for classical regression analysis. The independent variables for the regression analysis, the X terms, are also

not truly independent in a statistical sense. Errors can therefore result if one attempts to assign confidence limits on the rate coefficients arriving at erroneous conclusions. The "fit" of the predicted concentrations vs. space-time to the experimental data was therefore determined by comparison. However, the criterion of the comparison was strict in the following sense. If the chemistry indicated by the kinetic model was acceptable, and the kinetic model represented the trends of the experimental data, the model was considered to "fit" the data. On the other hand, if the chemistry of a proposed model did not agree with the experimental observations or the kinetic model did not predict trends of the experimental data, the model was rejected.

Two kinetic models were developed using the above solution techniques. The first is a basic model that was arrived at by testing many variations in the HJB.KINETIC.FIT routine until all positive rate constants were obtained and the chemistry was adequate but somewhat restrictive on the model for future work. Therefore, a more complete model was developed by the pattern search routine incorporating all of the chemistry observed in the experimental results. For this final model, activation energies were calculated by a pattern search which rapidly converged using the temperature-concentration data and base rate constants from the 661°K space-time kinetic model. These activation energy results were checked with the space-time-concentration data at 633°K. The next three sections present the kinetic models developed from application of the mathematical techniques discussed to the experimental data.

ii) Basic Model

The first step in obtaining the basic model was to estimate concentration vs. space-time data at equal space-time intervals from the experimental data as was discussed and shown in Figure 5.1. Using the 661°K data, the adjusted concentrations were determined and are listed in Table 5.1. In order to perform the matrix calculations, the code numbers for the compound groups were changed so that no zero rows were present. The compound groups corresponding to the new code numbers are listed in Table 5.2. Fluorene was combined with methylfluorene because it should proceed along the same reaction paths as fluorene, its parent structure. Compound group 5 of the original listing was not found to be a product of the decalin/fluorene reaction so it was eliminated. The kinetic model arrived at after many trials is shown in Figure 5.2 using the parent structures without substitution for each compound group. The decalin and tetralin reactions are separated for clarity. The reaction equations account for the continued reaction of tetralin from the decalin/fluorene reaction. The brackets indicate that both products are formed from the path pointing to the bracket. This is also accounted for in the model equations.

This overall scheme is broken down for each reaction as listed in Table 5.3 and from these reactions, the differential equations were written as presented in Table 5.4. Solving these equations for the rate coefficients by the HJB method with the Gauss-Jordan routine yields the rate coefficients listed in Table 5.5. Finally, input of the differential equations to LSODE with the rate coefficients, generates the predicted concentration vs space-time curves shown with the experimental data in Figures 5.3, 5.4, 5.5, and 5.6.

TABLE 5.1

Concentration for Equal Space-time Intervals at 661°K.

Space-time/s	Compound Group Concentration/kg-mole/m^3 x 10^5					
	ALK	CPT	CHX	BZ	DMOHP	TD
0	0.0	0.0	0.0	0.6	0.2	217.5
1	33.0	11.5	5.0	20.0	12.5	222.0
2	78.0	29.5	6.5	52.3	23.5	210.0
3	110.0	42.0	10.1	82.0	37.0	209.0
4	113.0	43.5	10.3	92.3	44.5	196.0
5	116.0	45.5	10.6	103.9	52.0	184.0

Space-time/s	Compound Group Concentration/kg-mole/m^3 x 10^5					
	CD	TT	IN	NAP	BIP	FLS
0	341.7	8.1	1.2	1.4	6.2	104.1
1	246.7	6.0	12.5	13.0	11.5	69.1
2	168.3	6.0	21.0	21.0	13.4	52.2
3	110.0	6.6	35.0	25.0	15.2	49.1
4	71.7	6.4	40.0	28.0	17.4	49.4
5	33.3	6.0	46.0	31.0	19.2	49.7

TABLE 5.2

Compound Group Code for Kinetic Model

Compound Number	Code Name	Structure Type
1	ALK	alkanes
2	CPT	cyclopentanes
3	CHX	cyclohexanes
4	BZ	benzenes
5	DMOHP	dimethyloctahydropentalene
6	TD	trans-decalin
7	CD	cis-decalin
8	TT	tetralin
9	IN	indanes
10	NAP	naphthalenes
11	BIP	biphenyls
12	FLS	fluorene and methylfluorene

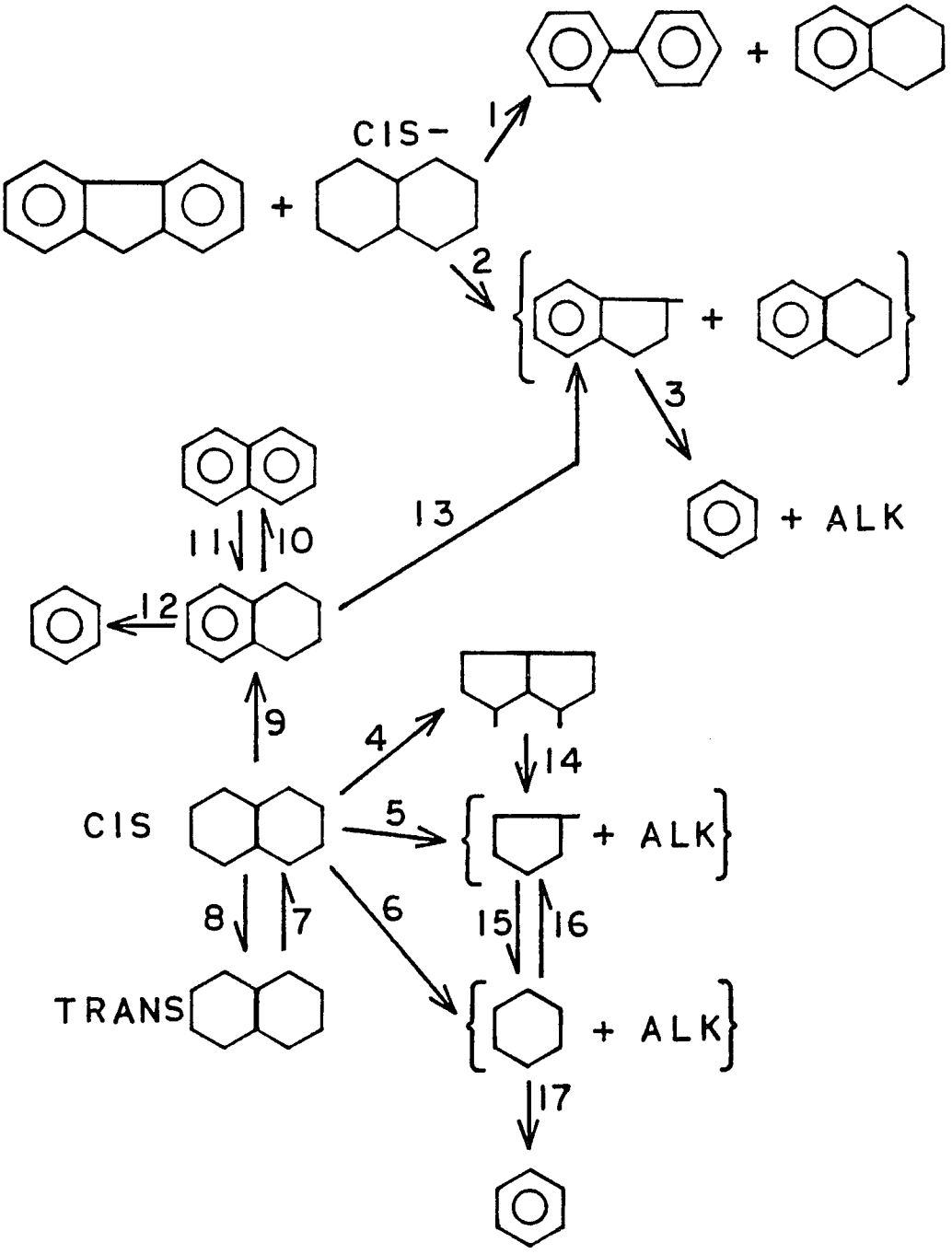


FIGURE 5.2 Basic Model Reaction Scheme Shown by Parent Structures. (Path numbers given by rate coefficient subscripts)

TABLE 5.3

Reactions of Basic Model in order of Rate Coefficient Number.

Rate Coefficient No.	Reaction
1	FLS + CD → BIP + TT
2	FLS + CD → IN + TT
3	IN → BZ + ALK
4	CD → DMOHP
5	CD → CPT + ALK
6	CD → CHX + ALK
7	TD → CD
8	CD → TD
9	CD → TT
10	TT → NAP
11	NAP → TT
12	TT → BZ
13	TT → IN
14	DMOHP → CPT
15	CPT → CHX
16	CHX → CPT
17	CHX → BZ

TABLE 5.4

Differential Equations of Basic Model Reaction Scheme

$$\frac{dALK}{dt} = k_3(IN) + (k_5+k_6)(CD)$$

$$\frac{dCPT}{dt} = k_5(CD) + k_{14}(DMOHP) - k_{15}(CPT) + k_{16}(CHX)$$

$$\frac{dCHX}{dt} = k_6(CD) + k_{15}(CPT) - (k_{16} + k_{17})(CHX)$$

$$\frac{dBZ}{dt} = k_3(IN) + k_{12}(TT) + k_{17}(CHX)$$

$$\frac{dDMOHP}{dt} = k_4(CD) - k_{14}(DMOHP)$$

$$\frac{dTD}{dt} = k_8(CD) - k_7(TD)$$

$$\frac{dCD}{dt} = k_7(TD) - (k_4 + k_5 + k_6 + k_8 + k_9)(CD) - (k_1 + k_2)(CD)(FLS)$$

$$\frac{dTT}{dt} = (k_1 + k_2)(CD)(FLS) + k_9(CD) + k_{11}(NAP) - (k_{10} + k_{12} + k_{13})(TT)$$

$$\frac{dIN}{dt} = k_2(CD)(FLS) - k_3(IN) + k_{13}(TT)$$

$$\frac{dNAP}{dt} = k_{10}(TT) - k_{11}(NAP)$$

$$\frac{dBIP}{dt} = k_1(CD)(FLS)$$

$$\frac{dFLS}{dt} = -(k_1 + k_2)(CD)(FLS)$$

TABLE 5.5

Rate Coefficients Determined for Basic Model at 661°K
Base Conditions

Coefficient No.	k, Rate Coefficient/$(s^{-1})^a$
1	2.1×10^{1} $m^3 \cdot kg \cdot mole^{-1} s^{-1}$
2	6.8×10^{1} $m^3 \cdot kg \cdot mole^{-1} s^{-1}$
3	8.2×10^{-3}
4	7.7×10^{-2}
5	1.0×10^{-1}
6	3.4×10^{-2}
7	7.4×10^{-2}
8	6.0×10^{-2}
9	2.0×10^{-2}
10	4.2
11	1.1
12	1.3
13	1.3×10^{-1}
14	1.2×10^{-1}
15	8.7×10^{-1}
16	1.9
17	2.0

a: unless otherwise noted for 2nd order terms where k [=] $m^3 \cdot kg \cdot mole^{-1} s^{-1}$

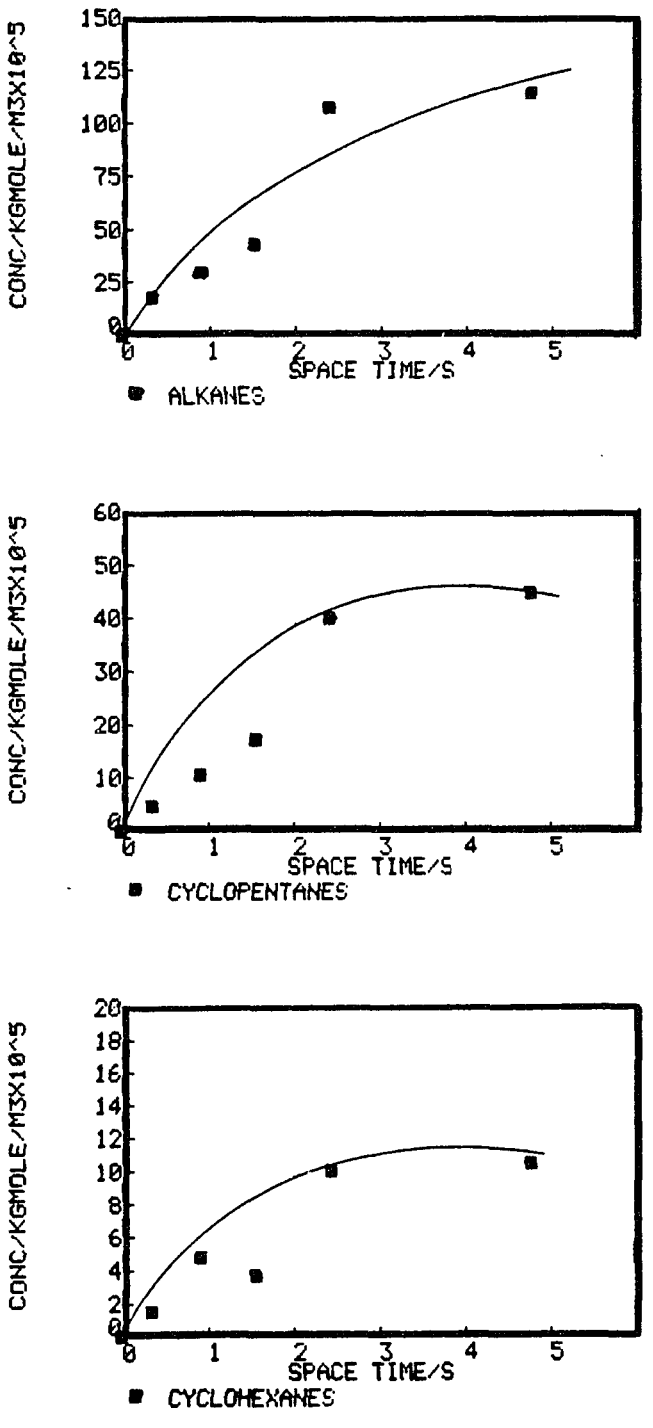


FIGURE 5.3 Basic Model Predicted Concentrations and Experimental Concentration Data at 661°K for ALK, CPT, and CHX.

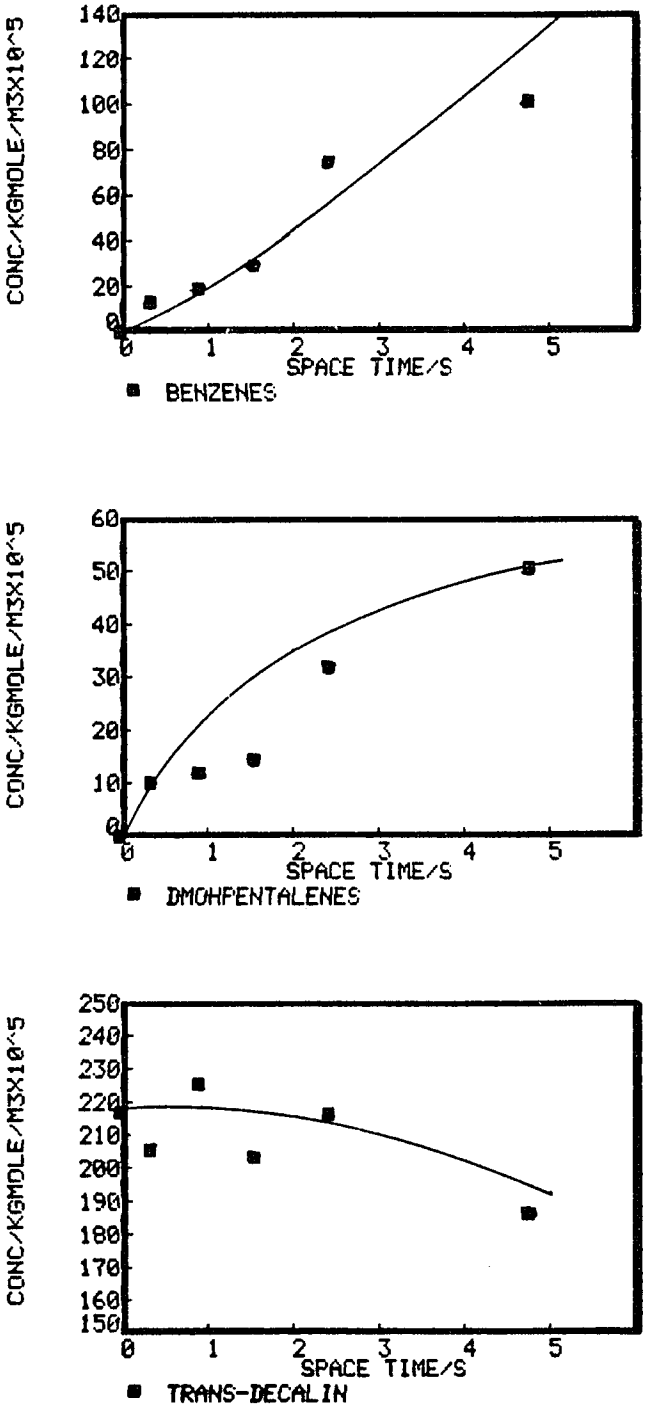
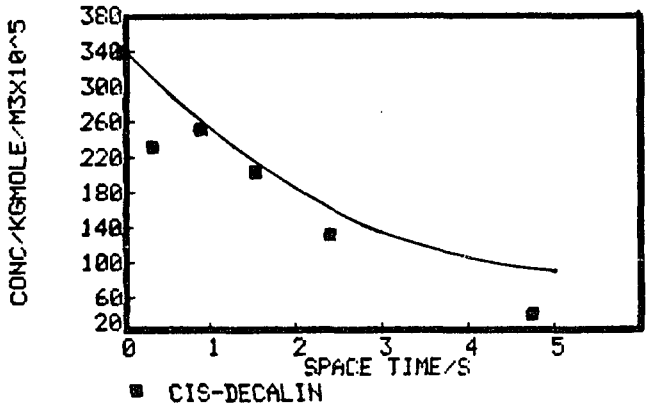
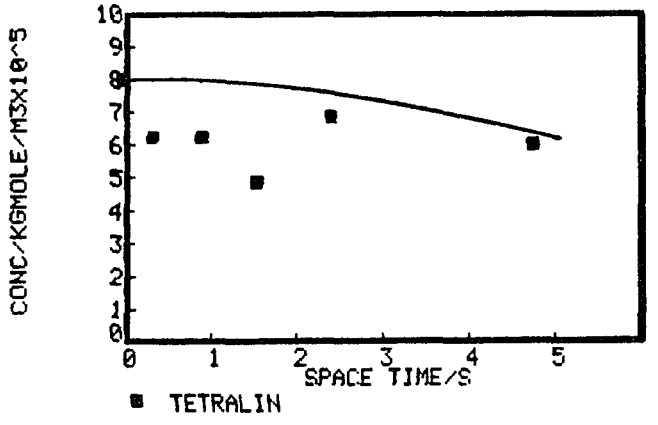


FIGURE 5.4 Basic Model Predicted Concentrations and Experimental Concentration Data at 661°K for BZ, DMOHP, and TD.





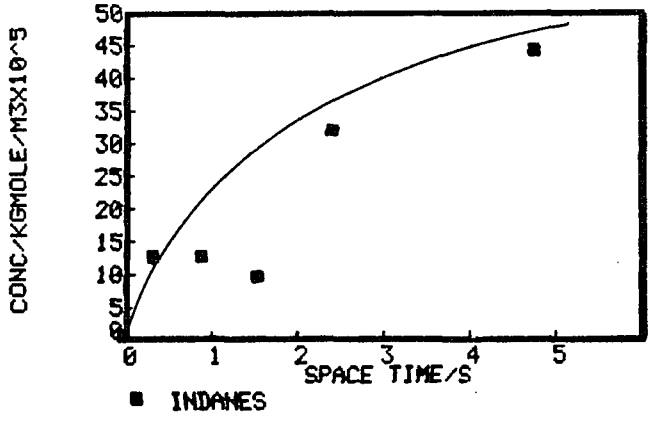


FIGURE 5.5 Basic Model Predicted Concentrations and Experimental Concentration Data at 661°K for CD, TT, and IN.

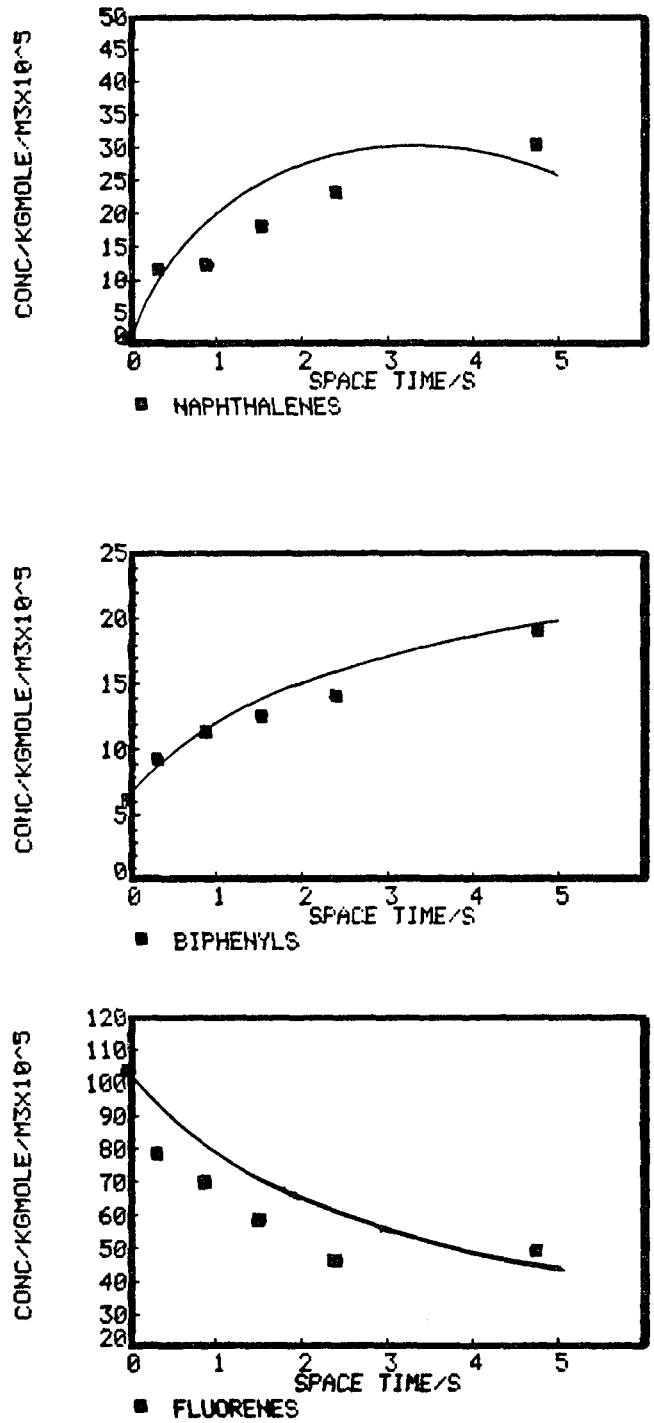


FIGURE 5.6 Basic Model Predicted Concentrations and Experimental Concentration Data at 661°K for NAP, BIP, and FLS.

This model provides a description of the kinetics with the requirement that for the fluorene reaction to occur, decalin must be dehydrogenated to tetralin which is then rapidly dehydrogenated further to naphthalenes or cracked to benzenes. A reversible reaction is included between cyclopentane and cyclohexane as was found by Selman (1972) to occur on zeolite catalysts. Since trans-decalin is fairly unreactive, it is included in a reversible reaction with cis-decalin only. The initial reaction of fluorene with cis-decalin is rapid in producing biphenyls which are non-reactive and indanes which proceed at a slow rate to benzenes and alkanes. Tetralin is also isomerized to indanes which further links the decalin/fluorene scheme. The results of this basic model work provided the basis for the development of the complex model.

iii) Complex Model

There are some problems with the chemistry of the basic model shown in Figure 5.2. First, the trend of the benzenes indicates it to be a secondary product while the data points show it to be initially formed as well as possibly being a secondary product. This is because the slope appears to be nonzero at t=0. The only source of initial benzene available is from the cracking of both sides of the central ring of fluorene. Therefore the reaction:

$$FL + CD \rightarrow 2\ BZ + TT$$

must be included. Secondly, all hydrogenation reactions should be restricted to require decalin for hydrogenation to occur because the effect of hydrogen pressure was negligible from 8.2 to 35.8 bar. This was tested in the reversible reaction of:

TT ↔ NAP

but was found not to fit the data. Therefore, the tetralin reaction is essentially irreversible and rapid to naphthalenes under the conditions of the study. Finally, the reaction of cis-decalin to DMOHP should be a reversible isomerization followed by isomerization and dehydrogenation of DMOHP to indanes and cracking of DMOHP to cyclopentanes and alkanes. Isomerization and cracking of DMOHP would also produce cyclohexane and alkanes. This change in the scheme of the DMOHP reaction is to account for the fact that the GC/MS analysis could not distinguish between the structure of DMOHP and that of saturated indanes and that both are possible in the reaction. With these adjustments to the basic model included, the complex model shown in Figure 5.7 was tested. As was shown for the basic model, the brackets clarify the scheme and the continued reaction of tetralin is accounted for in the model equations. The differential equations for the model are listed in Table 5.6. The pattern search routine was used, and after optimization, the rate coefficients were determined as listed in Table 5.7 for each reaction. The predicted concentrations with space-time are shown in Figures 5.8, 5.9, 5.10, and 5.11.

The same pattern search technique was used for the concentration vs. space-time data in Table 5.8 for 633°K which has been adjusted to equal space-time intervals. Rate coefficients for the same complex model were determined at 633°K as listed in Table 5.9 and used in the LSODE routine to produce the predicted curves shown in Figures 5.12, 5.13, 5.14, and 5.15.

The complex model was developed to account for the overall chemistry in hydrocracking fluorene with constraints of the observed

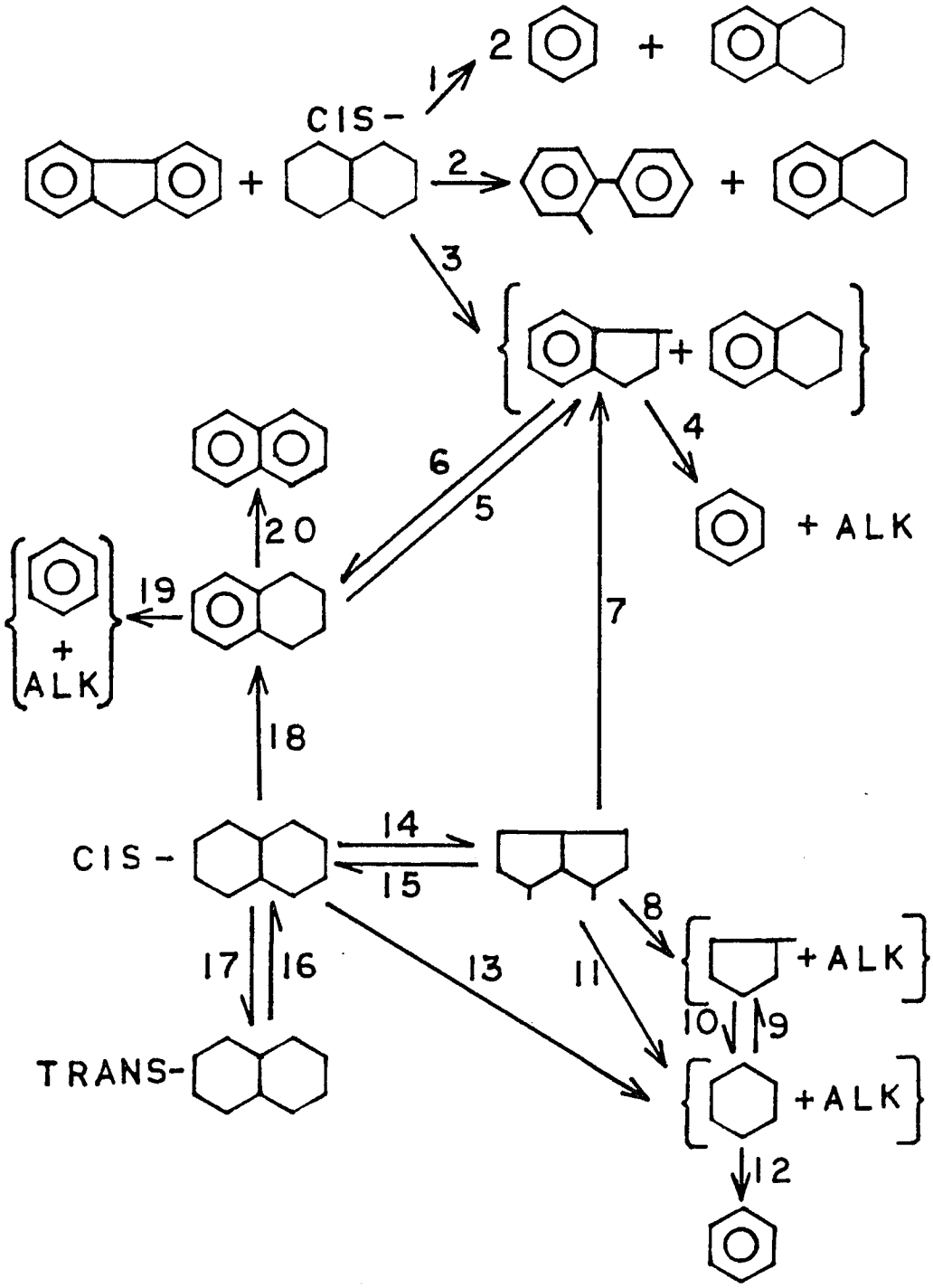


FIGURE 5.7 Complex Model Reaction Scheme Shown by Parent Structures of Compound Groups. (Numbers indicate corresponding rate coefficients)

TABLE 5.6

Differential Equations of Complex Model Reaction Scheme

$$\frac{dALK}{dt} = k_4(IN) + (k_8 + k_{11})(DMOHP) + k_{13}(CD) + k_{19}(TT)$$

$$\frac{dCPT}{dt} = k_8(DMOHP) + k_9(CHX) - k_{10}(CPT)$$

$$\frac{dCHX}{dt} = k_{10}(CPT) - (k_9 + k_{12})(CHX) + k_{11}(DMOHP) + k_{13}(CD)$$

$$\frac{dBZ}{dt} = 2k_1(CD)(FLS) + k_4(IN) + k_{12}(CHX) + k_{19}(TT)$$

$$\frac{dDMOHP}{dt} = k_{14}(CD) - (k_7 + k_8 + k_{11} + k_{15})(DMOHP)$$

$$\frac{dTD}{dt} = k_{17}(CD) - k_{16}(TD)$$

$$\frac{dCD}{dt} = k_{15}(DMOHP) + k_{16}(TD) - (k_1 + k_2 + k_3)(CD)(FLS) - (k_{13} + k_{14} + k_{17} + k_{18})(CD)$$

$$\frac{dTT}{dt} = (k_1 + k_2 + k_3)(CD)(FLS) + k_6(IN) + k_{18}(CD) - (k_5 + k_{19} + k_{20})(TT)$$

$$\frac{dIN}{dt} = k_3(CD)(FLS) + k_5(TT) + k_7(DMOHP) - (k_4 + k_6)(IN)$$

$$\frac{dNAP}{dt} = k_{20}(TT)$$

$$\frac{dBIP}{dt} = k_2(CD)(FLS)$$

$$\frac{dFLS}{dt} = -(k_1 + k_2 + k_3)(CD)(FLS)$$

TABLE 5.7

Rate Coefficients of Complex Model at 661°K

Coefficient No.	$k/(s^{-1})^a$	Reaction Path
1	2.5×10^{1} $m^3 kg \cdot mole^{-1} s^{-1}$	FLS + CD → 2BZ + TT
2	2.1×10^{1} $m^3 kg \cdot mole^{-1} s^{-1}$	FLS + CD → BIP + TT
3	7.2×10^{-3} $m^3 kg \cdot mole^{-1} s^{-1}$	FLS + CD → IN + TT
4	3.2×10^{-21}	IN → BZ + ALK
5	2.9	TT → IN
6	7.9×10^{-1}	IN → TT
7	2.4×10^{-1}	DMOHP → IN
8	2.8×10^{-17}	DMOHP → CPT + ALK
9	1.4×10^{1}	CHX → CPT
10	3.1	CPT → CHX
11	5.2×10^{-18}	DMOHP → CHX + ALK
12	7.8×10^{-2}	CHX → BZ
13	7.6×10^{-2}	CD → CHX + ALK
14	7.2×10^{-2}	CD → DMOHP
15	1.1×10^{-17}	DMOHP → CD
16	9.2×10^{-2}	TD → CD
17	7.7×10^{-2}	CD → TD
18	8.4×10^{-2}	CD → TT
19	2.0	TT → NAP
20	1.2	TT → BZ + ALK

a: unless otherwise noted where 2nd order terms have k [=] $m^3 \cdot kg \cdot mole^{-1} \cdot s^{-1}$.

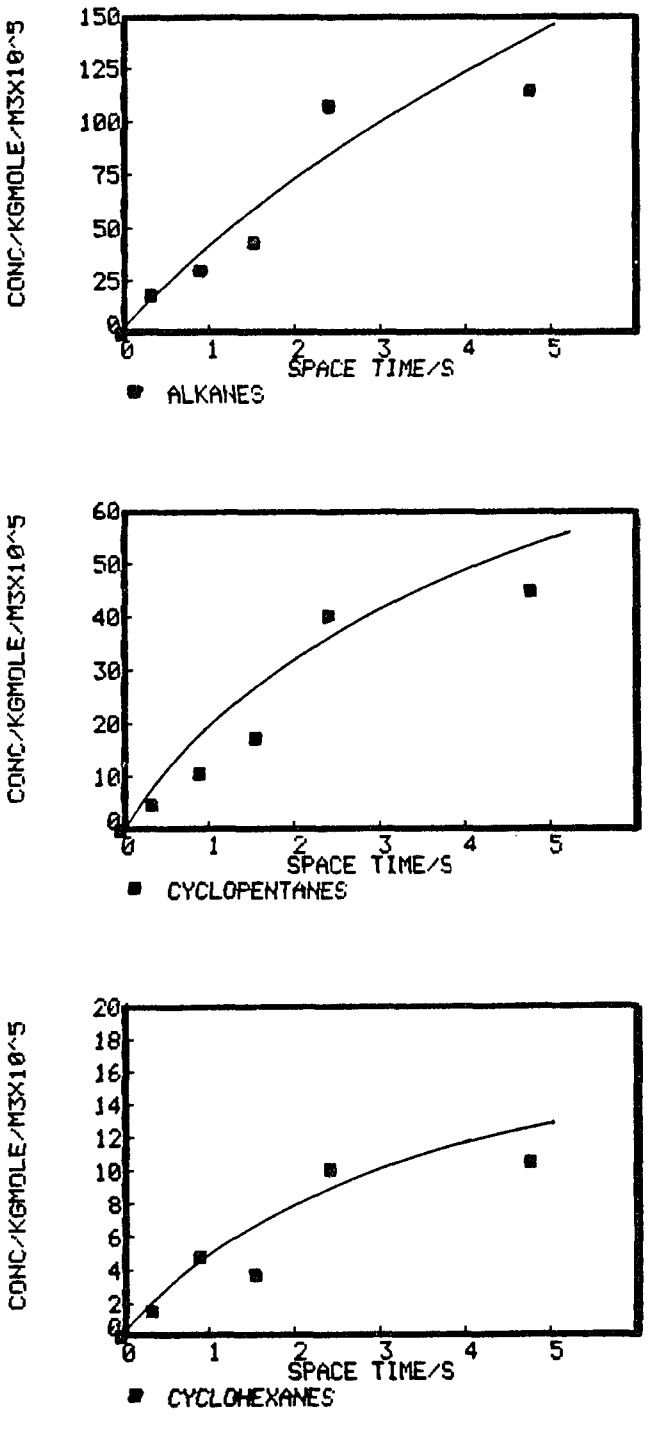
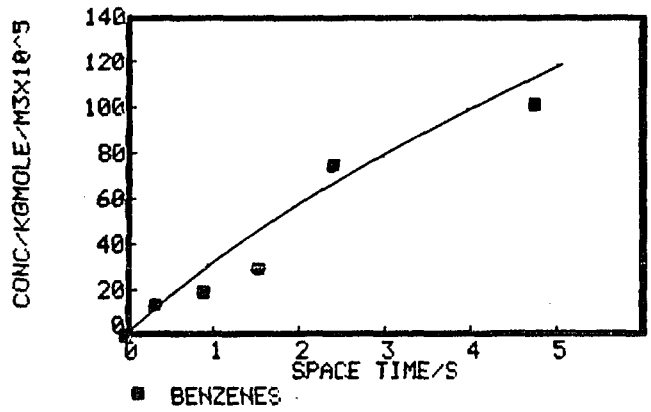
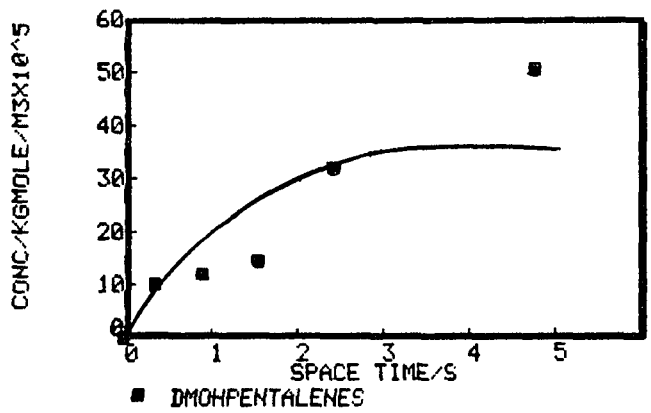


FIGURE 5.8 Complex Model Predicted Concentrations and Experimental Concentration Data at 661°K for ALK, CPT, and CHX.





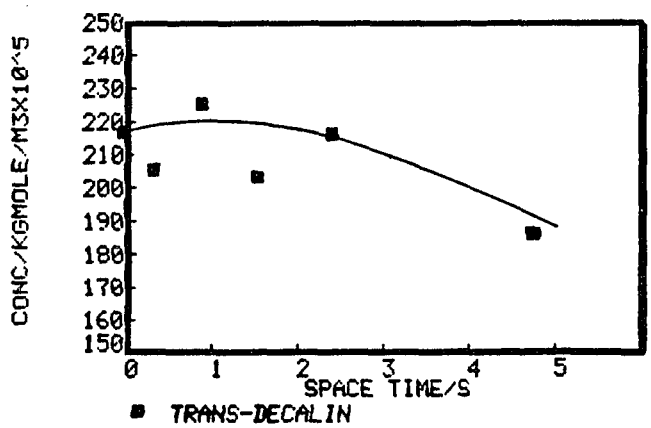


FIGURE 5.9 Complex Model Predicted Concentrations and Experimental Concentration Data at 661°K for BZ, DMOHP, and TD.

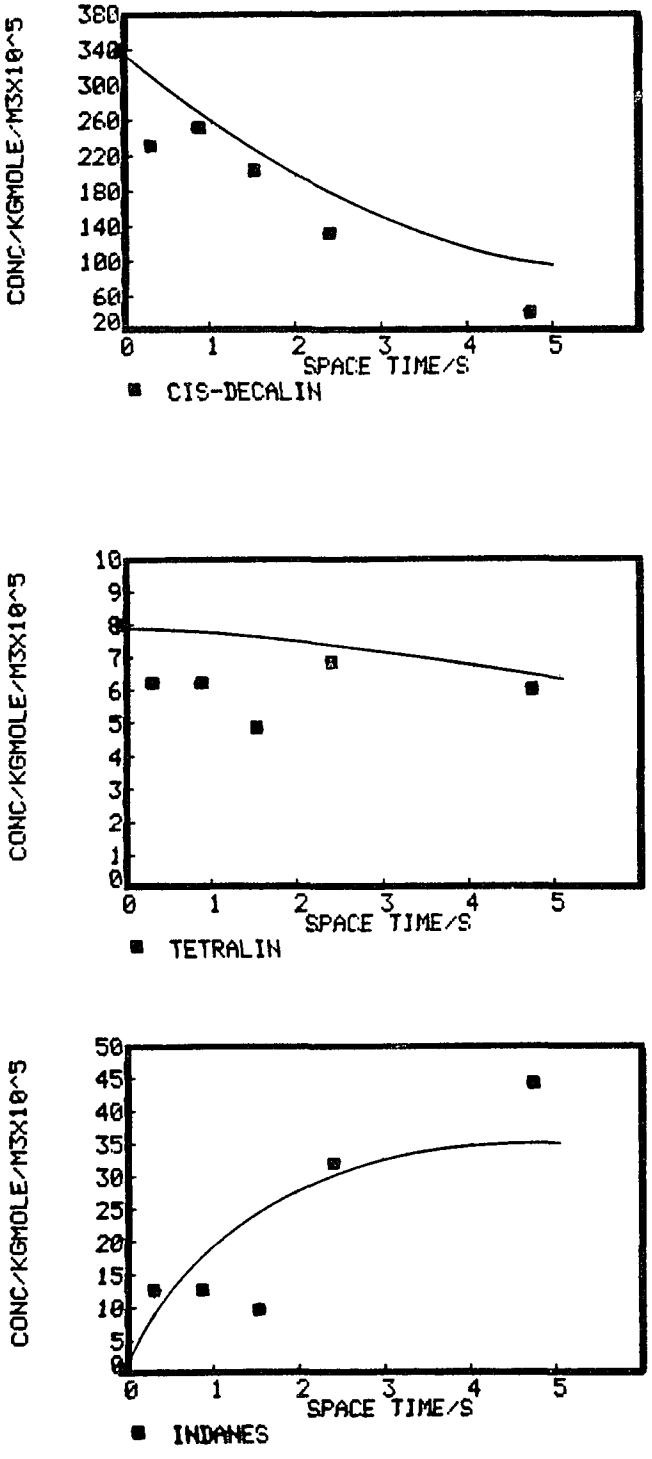


FIGURE 5.10 Complex Model Predicted Concentrations and Experimental Concentration Data at 661°K for CD, TT, and IN.

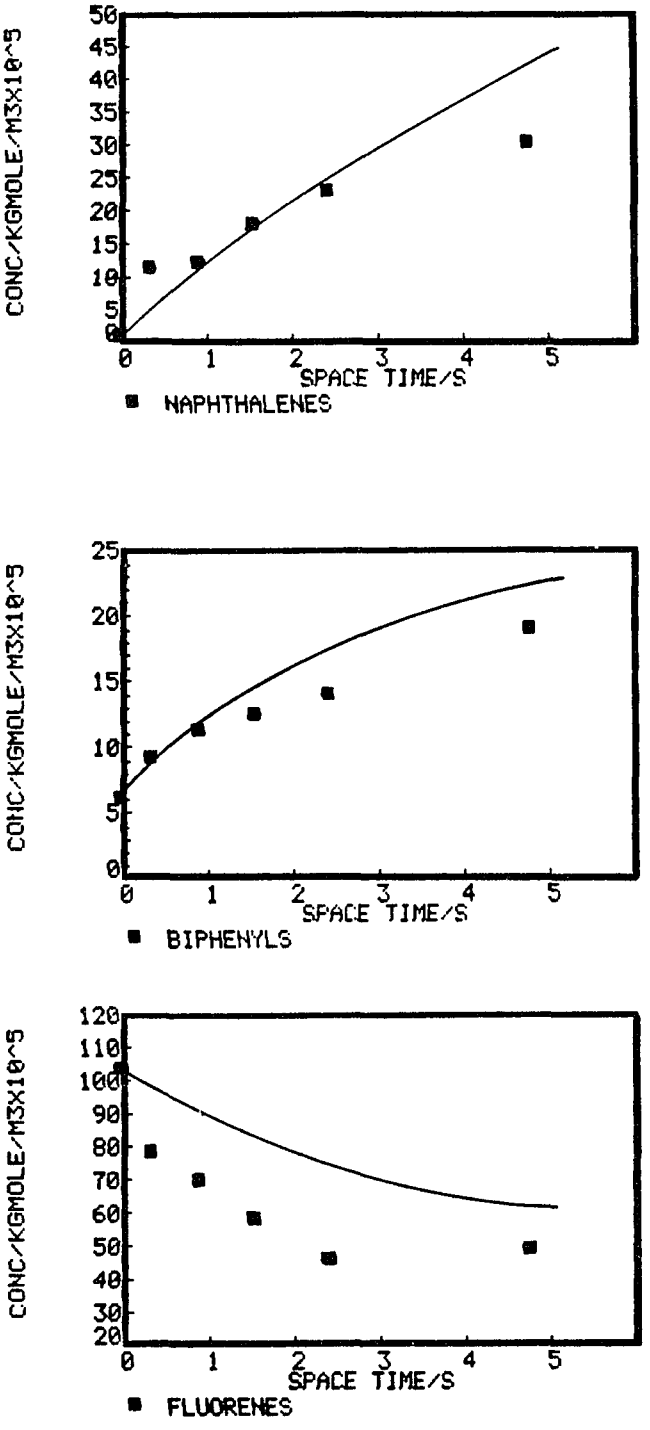


FIGURE 5.11 Complex Model Predicted Concentrations and Experimental Concentration Data at 661°K for NAP, BIP, and FLS.

TABLE 5.8

Concentration for Equal Space-Time Intervals at 633°K

Space-time/s	Compound Group Concentration/kg-mole/m^3 x 10^5					
	ALK	CPT	CHX	BZ	DMOHP	TD
0	0.0	0.0	0.0	0.6	0.2	227.1
1	23.0	8.1	2.1	28.8	17.3	242.0
2	40.0	14.7	3.8	55.0	33.6	251.0
3	48.0	19.7	5.1	81.2	58.2	253.0
4	52.0	21.7	5.7	82.5	58.2	251.0
5	53.8	23.4	6.2	80.0	55.5	248.0

Space-time/s	Compound Group Concentration/kg-mole/m^3 x 10^5					
	CD	TT	IN	NAP	BIP	FLS
0	356.7	8.4	1.2	1.4	6.5	108.7
1	265.0	7.6	11.5	11.3	15.4	94.0
2	180.0	7.7	18.8	17.0	21.3	83.5
3	110.0	7.7	24.0	21.2	25.0	77.5
4	95.0	7.6	26.9	22.5	24.6	73.0
5	100.0	7.5	29.2	22.0	24.2	72.0

TABLE 5.9

Rate Coefficients of Complex Model at 633°K

Coefficient No.	$k/(s^{-1})^a$	Reaction Path
1	3.1×10^{1} $m^3 kg \cdot mole^{-1} s^{-1}$	FLS + CD → 2BZ + TT
2	2.4×10^{1} $m^3 kg \cdot mole^{-1} s^{-1}$	FLS + CD → BIP + TT
3	9.0×10^{-15} $m^3 kg \cdot mole^{-1} s^{-1}$	FLS + CD → IN + TT
4	2.3×10^{-1}	IN → BZ + ALK
5	2.4	TT → IN
6	7.5×10^{-1}	IN → TT
7	1.2×10^{-1}	DMOHP → IN
8	3.4×10^{-19}	DMOHP → CPT + ALK
9	1.9	CHX → CPT
10	6.9×10^{-2}	CPT → CHX
11	1.8×10^{-1}	DMOHP → CHX + ALK
12	2.9×10^{-1}	CHX → BZ
13	9.7×10^{-3}	CD → CHX + ALK
14	1.0×10^{-1}	CD → DMOHP
15	5.5×10^{-17}	DMOHP → CD
16	3.9×10^{-2}	TD → CD
17	8.1×10^{-2}	CD → TD
18	9.7×10^{-3}	CD → TT
19	9.1×10^{-2}	TT → NAP
20	7.7×10^{-1}	TT → BZ + ALK

a: unless otherwise noted where 2nd order terms have k [=] $m^3 \cdot kg \cdot mole^{-1} \cdot s^{-1}$.

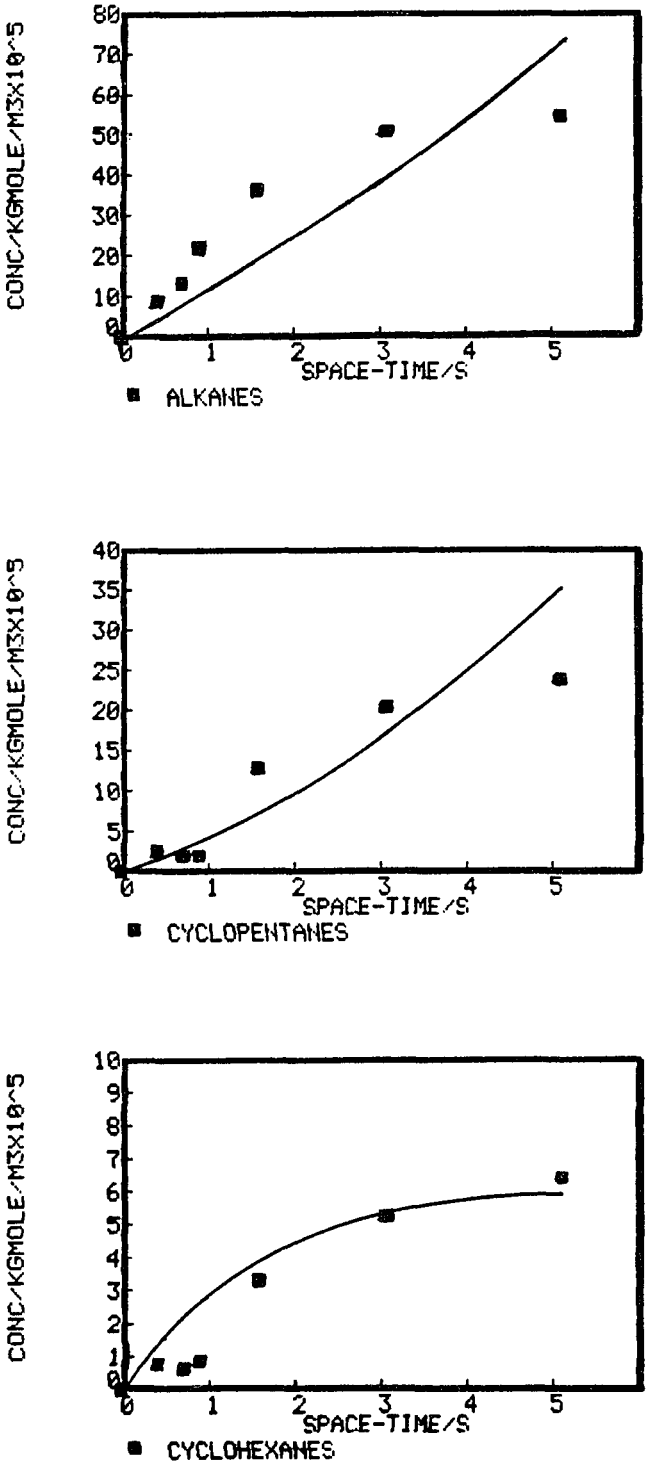


FIGURE 5.12 Complex Model Predicted Concentrations and Experimental Concentration Data at 633°K for ALK, CPT, and CHX.

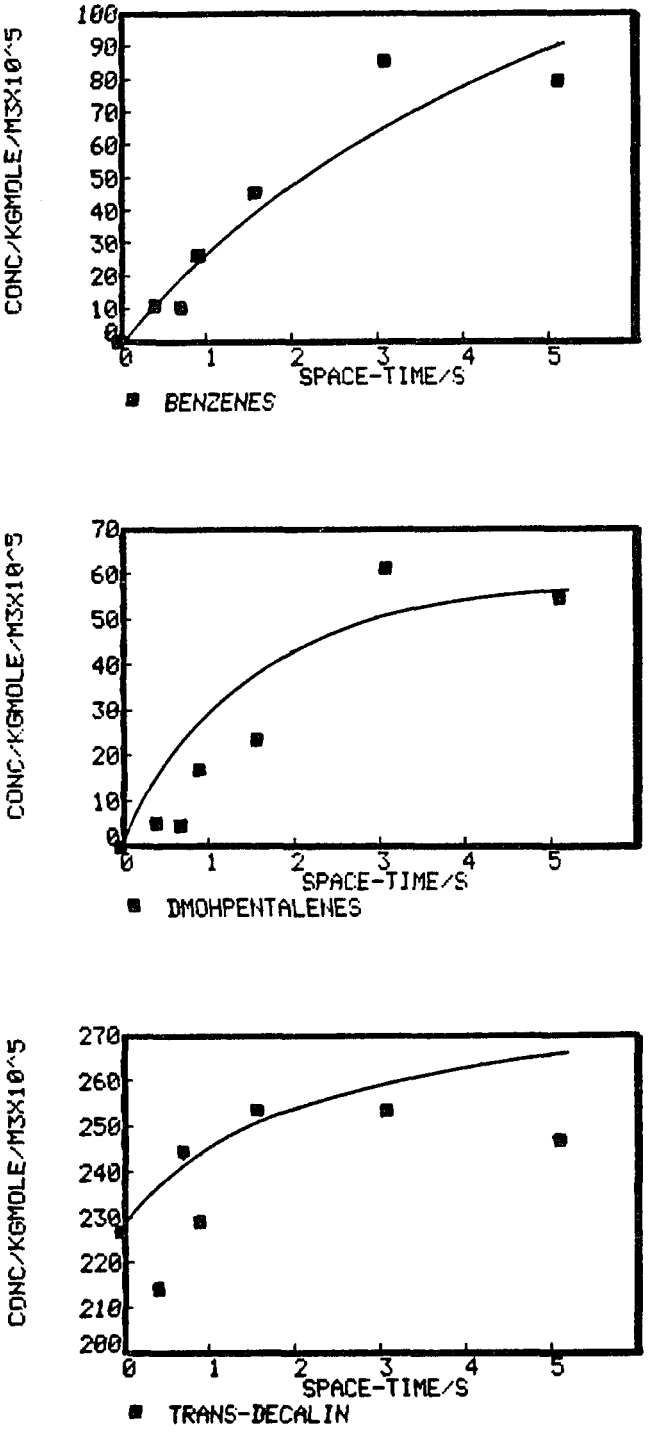


FIGURE 5.13 Complex Model Predicted Concentrations and Experimental Concentration Data at 633°K for BZ, DMOHP, and TD.

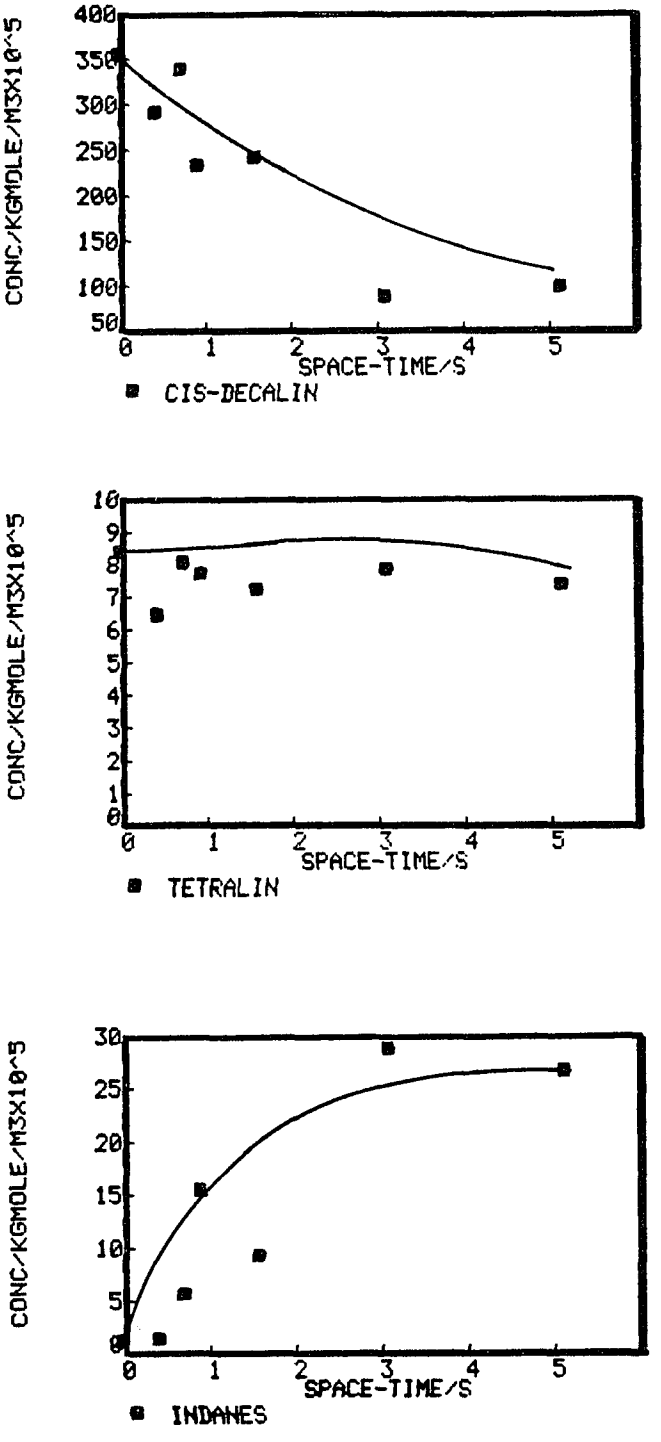


FIGURE 5.14 Complex Model Predicted Concentrations and Experimental Concentration Data at 633°K for CD, TT, and IN.

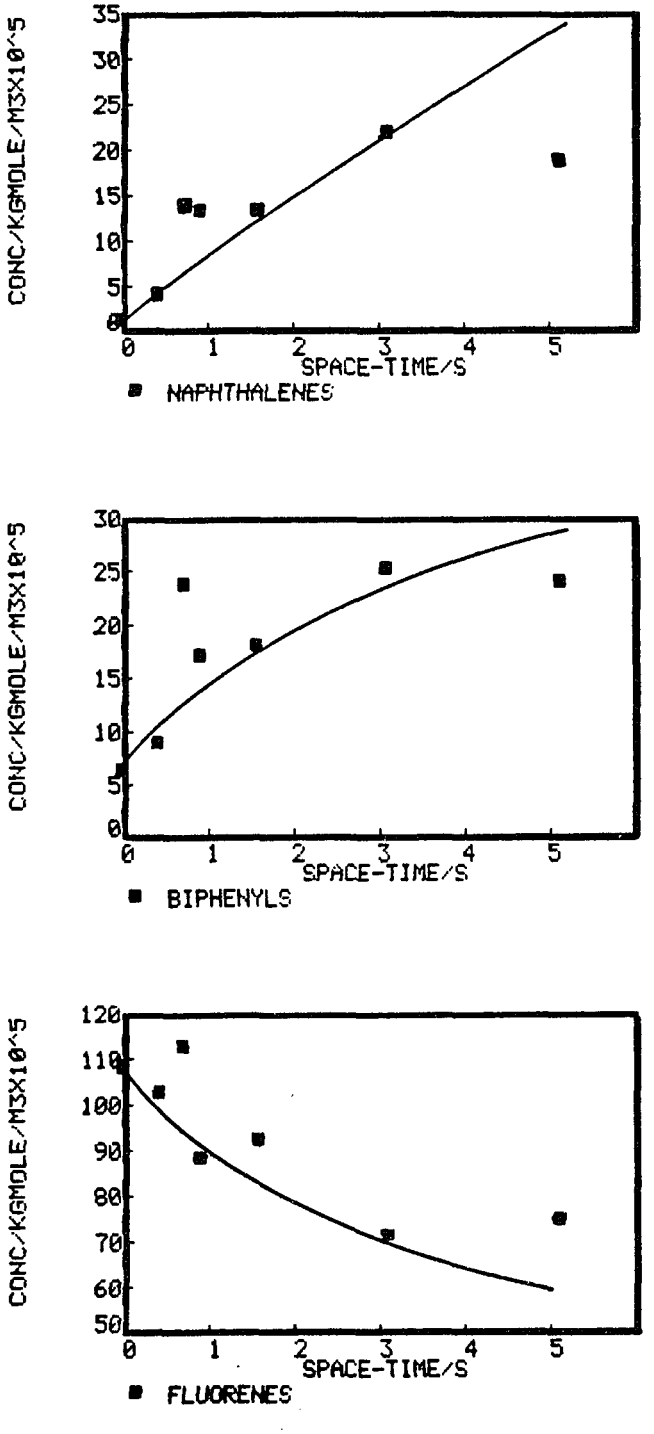


FIGURE 5.15 Complex Model Predicted Concentrations and Experimental Concentration Data at 633°K for NAP, BIP, and FLS.

experimental results. The complex model represents a compromise between the basic model and much more complex models that could be developed if all the assumptions were relaxed and the chemistry was completely understood. Therefore, analysis of the fit of the complex model should be make taking into account the simplifications made in development, i.e., grouping compounds, applying pseudo-homogeneous kinetics, neglecting coking and deactivation, and the uncertainty of the many possible routes of light hydrocarbon production. In such complex kinetic schemes, as discussed by Gardiner (1972), many times only the overall reaction rates can be determined with little knowledge obtained as to the makeup of the individual reactions. The two kinetic models presented have provided much more insight into the reaction of a model coal derived liquid in a donor solvent than just overall reaction rates. Both models show the interactions of the donor solvent and fluorene and allow for a general reaction mechanism to be proposed when coupled with the accepted theory of reactions on metal loaded zeolites.

iv) Activation Energy

As a final study of the proposed scheme of the complex model, activation energies for the reactions were estimated as a measure of the relative ease of reaction for each path. The Arrhenius relationship discussed in Chapter IV is only strictly valid for single reactions (Froment and Bischoff, 1979) which is not the case under study. However, it is common practice and by using the temperature-concentration data as listed in Table 5.10, a method was developed to obtain an estimate of activation energies as this accounts for the temperature dependency of the reaction and allows for prediction of concentrations at temperature other than base conditions (661°K).

TABLE 5.10

Concentration of Product Compound Groups as a Function of Temperature at a Space-time of Approximately 5 s from Temperature Series Experimental Runs.

	Compound Group Concentration/kg-mole/m^3 x 10^5						
T/°K	ALK	CPT	CHX	BZ	DMOHP	TD	CD
622.6	37.1	14.2	4.3	71.0	48.3	242.4	118.9
632.8	54.7	23.9	6.4	80.0	54.6	246.9	100.7
639.5	118.7	41.8	10.7	105.2	51.2	210.9	73.2
649.8	159.1	47.1	13.8	123.2	57.9	194.8	36.3
655.0	181.5	65.8	16.1	108.3	48.3	168.3	27.6
661.0	115.3	45.2	10.5	102.1	50.7	186.7	42.8
667.0	241.4	53.1	12.1	113.4	44.7	171.8	29.8
672.6	118.1	40.0	7.7	82.8	32.4	187.4	79.3
677.7	161.2	37.7	8.1	83.7	34.5	189.4	70.0
683.5	192.8	29.7	6.8	84.8	38.3	147.0	28.1
688.2	266.0	46.1	8.0	127.9	19.0	154.6	67.6
694.5	158.1	16.0	4.2	77.7	24.6	167.7	87.9

	Compound Group Concentration/kg-mole/m^3 x 10^5				
T/°K	TT	IN	NAP	BIP	FLS
622.6	6.8	18.7	17.7	21.0	78.4
632.8	7.5	26.8	19.1	24.1	75.4
639.5	8.5	37.6	25.4	18.2	41.8
649.8	7.6	43.8	27.2	20.5	33.5
655.4	6.0	42.0	31.1	17.1	33.1
661.0	6.0	44.6	30.7	19.0	49.6
667.0	6.4	54.7	39.6	17.2	24.5
672.6	6.2	43.0	30.0	16.1	48.8
677.7	6.0	44.2	37.6	17.2	53.4
683.5	6.0	55.2	44.9	20.5	40.6
688.2	3.2	40.0	48.5	19.3	23.4
694.5	3.4	36.1	39.9	17.2	44.7

Rate coefficients for 633 and 661°K have been presented but application of only two points to the typical Arrhenius plot would be a poor estimate at best of E_A/R, the slope and resulting E_A. Higher confidence was placed on the 661°K rate coefficients than on the 633°K coefficients by comparison of the scatter of the concentration/space time experimental data. Therefore, the following technique was used employing the pattern search routine. Using the rate coefficients at 661°K, and an initial guess (10000 kcal/kg-mole) of E_A for each reaction, the Arrhenius equation may be solved for A_k, the frequency factor for each k_k as:

$$A_{k_{661}} = k_{k_{661}} e^{E_{A_k}/RT_{661}} \qquad 5.12$$

Now, with the kinetic model equations listed in Table 5.6, the rate coefficients may be replaced with the Arrhenius equation:

$$k_k = A_{k_{661}} e^{-E_{A_k}/RT} \qquad 5.13$$

with the guessed value of E_{Ak} and calculated value of A_k inserted and k_k calculated for each temperature corresponding to the concentration-temperature series.

This was done in the pattern search routine ACTIV listed in Appendix 4 with the following optimization performed. The numerical integration of the concentration terms R_{ijk} is performed in one step from 0 to 5 s for each temperature listed in Table 5.10. To optimize the estimated activation energies the routine adjusts the step size around E_{Ak} and minimizes the sum of squares of the weighted deviations of the changes in concentration from 622 to 694°K. In other words, if the guessed activation energy and resulting frequency factor do not

supply a k_k at each temperature corresponding to the concentration data, the least squares criterion would not be at a minimum and a new value of E_{Ak} would be determined based on the step size function until minimization was established.

Since the integration routine requires initial concentrations for each temperature, the initial concentrations of each compound group at 661°K were adjusted to the run temperature assuming the ideal gas law was valid. These initial concentrations are listed in Table 5.11. Input to the ACTIV routine is then the initial concentrations, concentrations for each temperature at a space-time of 5 s and the rate coefficients at 661°K for each reaction. The optimum values as obtained by this routine are listed in Table 5.12 with the corresponding reaction.

These activation energies are in the typical range expected except for two problems. Activation energies for 5 reactions could not be determined based on the 661°K data. The reactions of:

IN → TT

DMOHP → CD

DMOHP → CPT + ALK

DMOHP → CHX + ALK

CD → CMOHP

did not result in activation energies being estimated due to either no effect, i.e., the guessed value of activation energy did not change or extremely small activation energies were found indicating no function of temperature.

These anomalies may be resolved when one considers the values of the rate coefficients as input data at 661°K. No change in E_A occurred

TABLE 5.11

Initial Concentration of Compound Groups as a Function of Temperature (space-time=0 s)

	Compound Group Concentration/kg-mole/m^3 x 10^5					
T/°K	ALK	CPT	CHX	BZ	DMOHP	TD
622.6	0.0	0.0	0.0	0.6	0.2	231.2
632.8				0.6	0.2	227.1
639.5				0.6	0.2	225.0
649.8				0.6	0.2	221.2
655.4				0.6	0.2	219.5
661.0	0.0	0.0	0.0	0.6	0.2	217.5
667.0				0.6	0.2	215.7
672.6				0.6	0.2	214.0
677.7				0.6	0.2	212.1
683.5				0.5	0.2	210.5
688.2				0.5	0.2	208.7
694.5	0.0	0.0	0.0	0.5	0.2	207.2

	Compound Group Concentration/kg-mole/m^3 x 10^5					
T/°K	CD	TT	IN	NAP	BIP	FLS
622.6	363.1	8.6	1.2	1.4	6.6	110.6
632.8	356.7	8.4	1.2	1.4	6.5	108.7
639.5	353.4	8.3	1.2	1.4	6.5	107.7
649.8	347.5	8.2	1.2	1.4	6.4	105.9
655.4	344.8	8.1	1.2	1.4	6.3	105.1
661.0	341.7	8.1	1.2	1.4	6.2	104.1
667.0	338.9	8.0	1.1	1.4	6.2	103.2
672.6	336.1	7.9	1.1	1.3	6.1	102.4
677.7	333.1	7.9	1.1	1.3	6.1	101.5
683.5	330.7	7.8	1.1	1.3	6.1	100.7
688.2	327.8	7.7	1.1	1.3	6.0	100.0
694.5	325.4	7.7	1.1	1.3	6.0	99.2

TABLE 5.12

Activation Energy by Reaction Path Based on 661°K Rate Coefficients

E_A/kcal/kg-mole	Reaction Path
14000	FLS + CD → 2BZ + TT
10000	FLS + CD → BIP + TT
15000	FLS + CD → IN + TT
20000	IN → BZ + ALK
20000	TT → IN
-	IN → TT
8000	DMOHP → IN
-	DMOHP → CPT + ALK
19000	CHX → CPT
8000	CPT → CHX
-	DMOHP → CHX + ALK
134000	CHX → BZ
28000	CD → CHX + ALK
-	CD → DMOHP
-	DMOHP → CD
16000	TD → CD
9000	CD → TD
36000	CD → TT
23000	TT → NAP
24000	TT → BZ + ALK

in the cases where the rate coefficients were very small and these made the effect of the exponential term negligible in the optimization after calculation of the frequency factor. This indicates that the optimization routine is not sensitive to the activation energies of these reactions. Finally, extremely small activation energies are a result of no temperature dependency for the reaction of:

$$IN \rightarrow TT$$

$$DMOHP \rightarrow CD$$

over the temperature range investigated. Certainly, this does not mean that there is not an activation energy for these reactions, but shows that the temperature range of these experiments had no effect on the rate of reaction, possibly due to experimental error. No other consistent explanation could be made for this problem assuming that these reactions do indeed take place.

To test the validity of the other 15 activation energies determined, frequency factors were calculated at 661°K and assuming that the frequency factors are constants, rate coefficients were calculated at 633°K as listed in Table 5.13 for the complex model in comparison with the 633°K space-time series results. Using the LSODE routine, concentration vs. space-time data was predicted for the model and compared to the 633°K experimental data as shown in Figures 5.16, 5.17, 5.18, and 5.19.

There are however, inconsistent results in the comparison of rate coefficients by the two methods. The coefficients of reaction paths 3, 4, 10, 11, and 12 are not within orders of magnitudes of each other for the two approaches. The following are offered as possible explanations for the inconsistent results.

TABLE 5.13

Rate Coefficients from Activation Energy using Frequency Factor at 661°K for 633°K

Rate Coefficient No.	$(k/s^{-1})^a$ from E_{act}	$(k/s^{-1})^a$ from 633°K space time series
1	1.6×10^{1} a	3.1×10^{1} a
2	1.3×10^{1} a	2.4×10^{1} a
3	4.4×10^{-3} a	9.0×10^{-15} a
4	1.6×10^{-21}	2.3×10^{-1}
5	1.5	2.4
6	7.9×10^{-1}	7.5×10^{-1}
7	1.8×10^{-1}	1.2×10^{-1}
8	2.0×10^{-17}	3.4×10^{-19}
9	7.2	1.9
10	2.3	6.9×10^{-2}
11	3.7×10^{-18}	1.8×10^{-1}
12	8.5×10^{-4}	2.9×10^{-1}
13	2.9×10^{-2}	9.7×10^{-3}
14	7.2×10^{-2}	1.0×10^{-1}
15	8.2×10^{-18}	5.5×10^{-17}
16	5.3×10^{-2}	3.9×10^{-2}
17	5.7×10^{-2}	8.1×10^{-2}
18	2.5×10^{-2}	9.7×10^{-3}
19	9.4×10^{-1}	9.1×10^{-2}
20	5.2×10^{-1}	7.7×10^{-1}

a: unless otherwise noted where 2nd order terms have k [=] $m^3 \cdot kg \cdot mole^{-1} \cdot s^{-1}$.

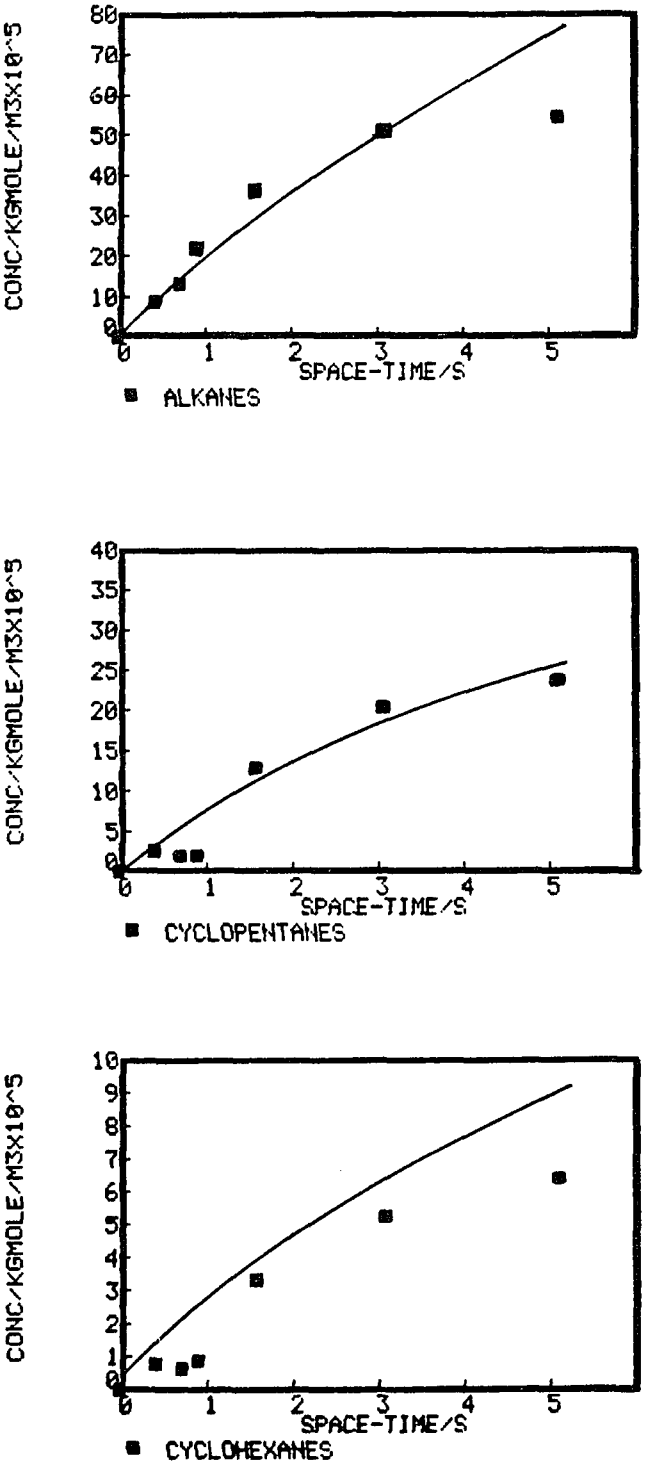


FIGURE 5.16 Complex Model Predicted Concentrations at 633°K From Estimation of Activation Energies (ALK, CPT, CHX).

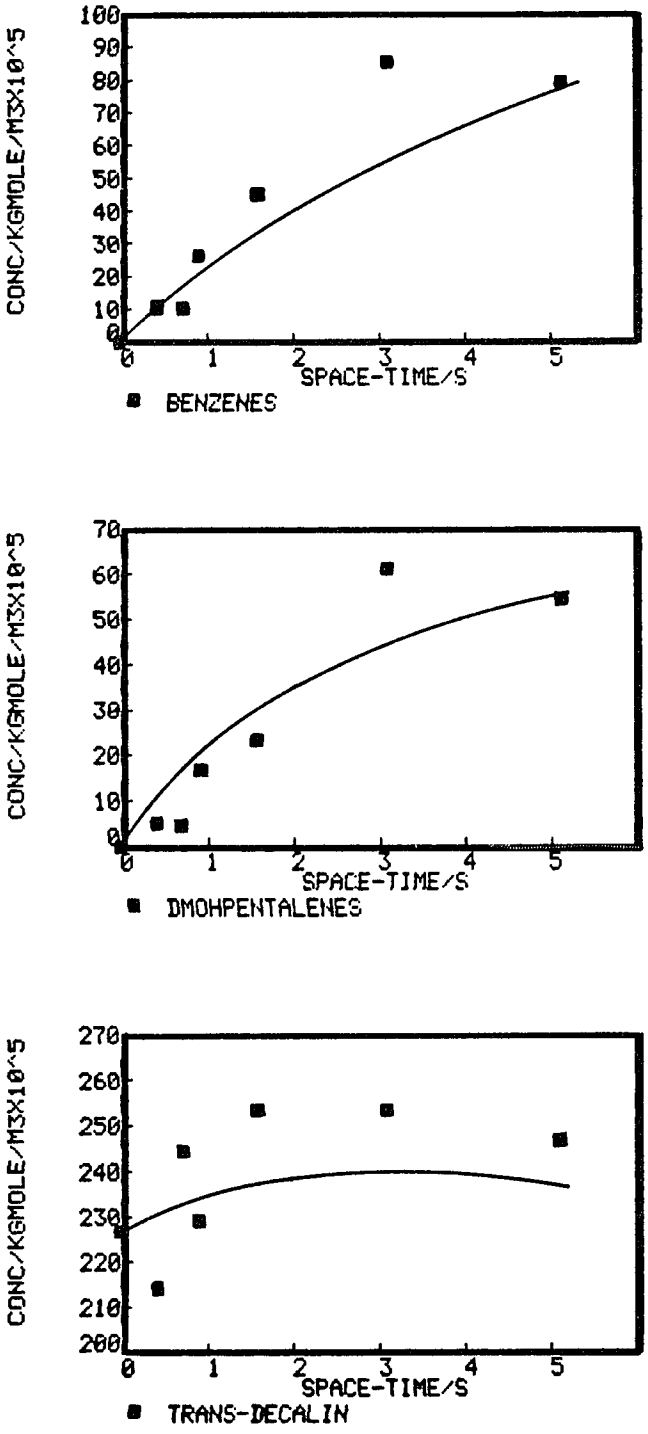


FIGURE 5.17 Complex Model Predicted Concentrations at 633°K From Estimation of Activation Energies (BZ, DMOHP, TD).

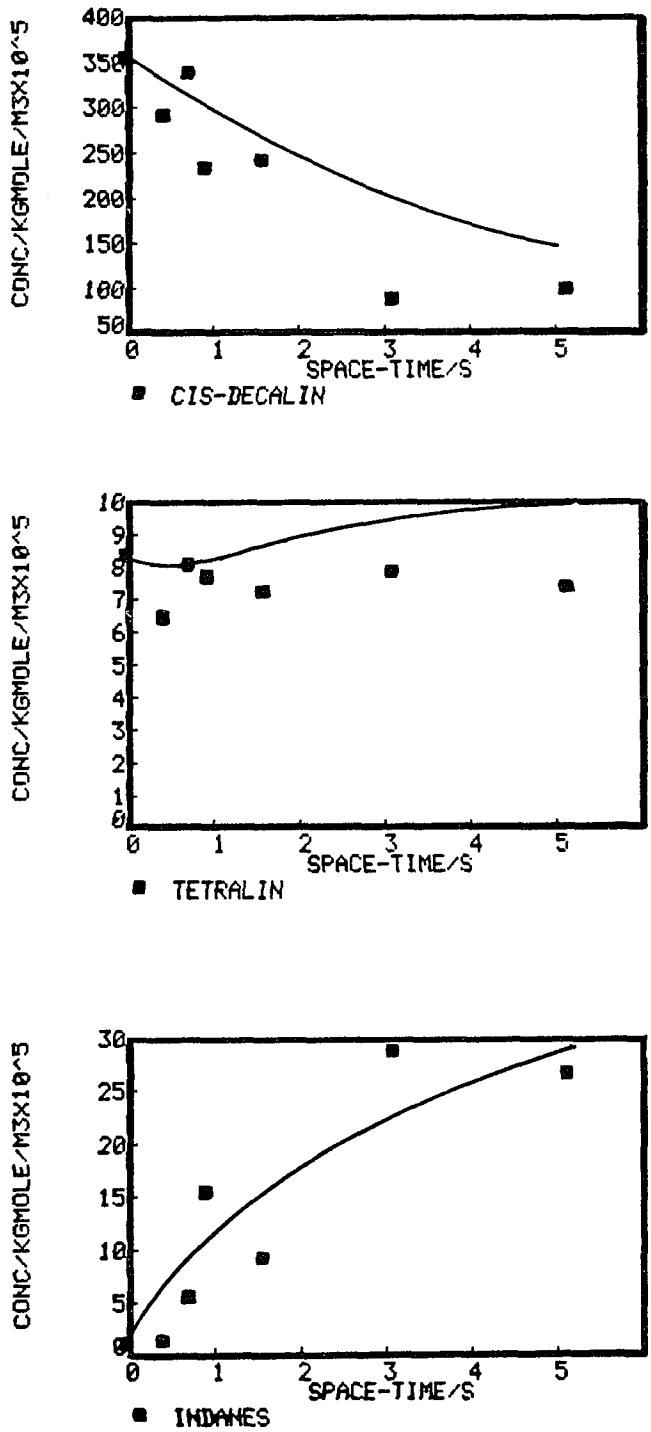
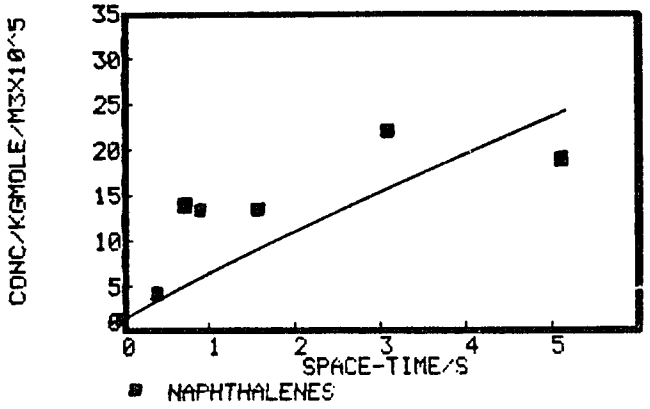
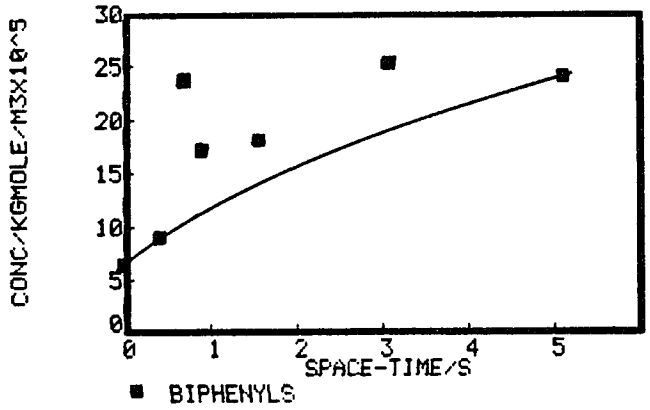


FIGURE 5.18 Complex Model Predicted Concentrations at 633°K From Estimation of Activation Energies (CD, TT, IN).





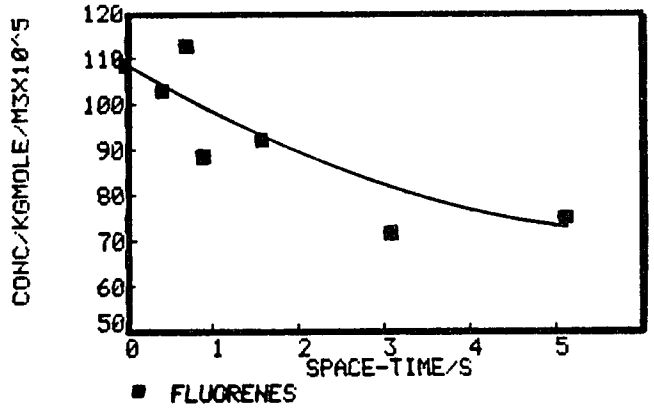


FIGURE 5.19 Complex Model Predicted Concentrations at 633°K From Estimation of Activation Energies (NAP, BIP, FLS).

1. Experimental error; i.e., the temperature runs were made during the study while the final product recovery system was under development, unlike the space-time runs where the product recovery technique was fully developed.

2. All of the activation energies were not determined for the reaction scheme from the pattern search and estimates were used for those not being optimized.

3. The temperature series concentration data was integrated from 0 to 5 seconds in one step, which is not as accurate as the integrals of the space-time data over 5 time step intervals.

4. The predicted concentration-space-time curves of both analyses represent the trends of the experimental data. This is because in combining the individual rate coefficients into the coefficients of the differential equations for the solution from LSODE, the majority of the terms are not affected by the differences of the two techniques, hence similar solutions are obtained.

Based on the explanations offered, more significance should be placed on the results of the space-time series for rate coefficients and the activation energies should be used only as a relative comparison of the effect of temperature on rate coefficients for the kinetic model.

v) Proposed Mechanism

In light of the discussion and assumptions made in arriving at the kinetic models, one cannot hope to propose a detailed reaction mechanism for this system. Due to lack of knowledge of the specific reactions on the surface sites where many compounds are interacting, only certain interactions are confirmed. It is perhaps best then to state the

mechanism as it was deduced from experimental observations and fit of the kinetic models to the data assuming an Eley-Rideal type mechanism is operative between fluorene and decalin. The steps observed are summarized below as the proposed reaction mechanism for fluorene, as a model of coal-derived liquids in the donor solvent decalin, over the Ni-Y zeolite catalyst.

1. The reaction is initiated by fluorene being adsorbed on the catalyst surface forming a reactive species. This adsorbed species is attacked by decalin in the gas phase and undergoes hydrogenation by hydrogen transfer from decalin.

2. Cracking of fluorene occurs by three routes; central ring cracking of both the phenyl-phenyl and the phenyl-methyl bonds to produce benzenes and cracking only the phenyl-methyl bond to produce biphenyls; and side ring cracking forming indanes.

3. Further cracking of the 5 member hydrogenated ring of indanes resulting in benzenes and also a reversible isomerization of the 5 member ring to 6 forming tetralin.

4. Four steps are operative in the cis-decalin reaction. The primary and essential one is the gas phase dehydrogenation to tetralin supplying hydrogen to fluorene located on the catalyst sites. Three other mechanisms of decalin reaction are isomerization and cracking; promoted by the acidic sites, and dehydrogenation directly on the metal sites forming tetralin.

5. In addition to the isomerization of DMOHP with cis-decalin, it undergoes a dehydrogenation function from the metal sites forming indanes.

6. The nickel sites promote hydrogenation/dehydrogenation and the acidic sites promote both cracking via carbonium ion mechanism routes and isomerization.

7. Molecular hydrogen serves to control coke formation during reaction and reduction of the metal before reaction.

To produce compounds typical of gasoline fractions from the model coal derived liquid component, fluorene, a complex reaction mechanism is involved with hydrogenation of fluorene occurring on the metal sites where hydrogen is supplied from dehydrogenation of decalin in the gas phase and then continuing the reaction by three cracking routes promoted by the acidic sites. Side reactions of decalin were isomerization, dehydrogenation directly on the metal sites, and cracking, producing both saturated and aromatic ring compounds and alkanes.

4) Literature Cited

Brignac, S.D., "A Reactor Study of Nickel Loaded Zeolites", M.S. Thesis, L.S.U. (1984).

Carnahan, B., H.A. Luther, and J.O. Wilkes, Applied Numerical Methods, J. Wiley, New York (1969).

Eley, D.D. and E.K. Rideal, Proc. R. Soc. London, Ser A., 178, 429-452 (1941).

Froment, G.F. and K.B. Bischoff, Chemical Reactor Analysis and Design, J. Wiley, New York (1979).

Gardiner, W.C., Jr., Rates and Mechanisms of Chemical Reactions, Benjamin/Cummings, Menlo Park (1972).

Hall, W.K., Chem. Eng. Prog. Symp. Ser., 63, 68 (1967).

Hill, C.G., Jr., An Introduction to Chemical Engineering Kinetics and Reactor Design, J. Wiley, New York (1978).

Himmelblau, D.M., C.R. Jones, and K.B. Bischoff, Ind. Eng. Chem. Fund., 6(4), 539 (1967).

Hindmarsh, A.C., ACM-SIGNUM Newsletter, 15 (4), 10 (1980).

Hougen, O.A. and K.M. Watson, Ind. Eng. Chem., 35, 529 (1943).

Langmuir, I., J. Am. Chem. Soc., 38, 221 (1916).

Langmuir, I., J. Am. Chem. Soc., 40, 1361 (1918).

Moore, C.F., C.L. Smith, and P.W. Murrill, "PATERN Search Program", L.S.U. (1969).

Selman, D.M., "Catalytic Reforming of Methylcyclopentane", Ph.D. Dissertation, L.S.U. (1972).

Voorhies, A., Jr., Ind. Eng. Chem., 37 (4), 318 (1945).

CHAPTER VI

Conclusions and Recommendations

1) Overall Conclusions

The hydrocracking of fluorene, acting as a model coal derived liquid component, has been investigated using decalin, a donor solvent, on a nickel loaded Y zeolite at typical hydrocracking conditions. During the course of this investigation, an existing reactor system, which was used previously for light hydrocarbon studies, was modified so that coal derived liquids could be processed. Included in this work was development of a material balance procedure and associated analytical techniques essential for the kinetic study.

Two kinetic models were formulated, based on results obtained from the qualitative experiments and analysis of the data from each quantitative experimental series. The kinetic study was based on application of pseudo-homogeneous rate expressions with concentration terms being expressed as compound groups. Including feedstocks, fifty compounds were identified in the product mixture, which was simplified by combining each compound of similar structure into a "compound group". No thermal, external mass transfer, or pore diffusion limitations were found, which indicated that the chemical reaction was the rate limiting step. However, configurational diffusion may cause the reaction to proceed only on the external surface of the catalyst. The Himmelblau-Jones-Bischoff method was used to determine rate coefficients by two solution techniques, Gauss-Jordan elimination and a pattern search. The pattern search routine proved to be more efficient in the analysis of different models since rate coefficients were constrained to be positive

and the results could be used in the differential equation solving program LSODE to obtain a solution to the differential equations.

The basic model developed for 661°K space-time data served as a starting point for the complex model which accounted for the chemistry of the reaction as understood at this time. Rate coefficients were determined for the basic model at 661°K and for the complex model at 633 and 661°K at a pressure of 14.8 bar. Predicted concentrations vs. space-time for both models were presented in comparison to the experimental data. These results represented a compromise between curve fits that could be obtained if the chemistry of the process was not accounted for, and the true kinetic model if each compound were treated separately knowing all of the chemistry involved. In other words, a purely mathematical approach must be tempered with application of known and observed chemistry of the reactions to arrive at a realistic model.

Activation energies were estimated for fifteen out of twenty of the complex model reaction pathways and should be considered only as a relative indication of the effect of temperature on the reaction rates for the model.

The effects of coking and deactivation were not accounted for in the kinetic model. However, it was found that coke formation was uniform and a function of catalyst exposure time. Regeneration of the coked catalyst returned it to a high activity indicating that nickel metal migration and agglomeration were not significant.

An overall reaction mechanism was proposed, based on the experimental results obtained, and accepted concepts of catalysis, accounting for the roles of hydrogen, decalin, and the catalyst sites in the hydrocracking of fluorene. The main points of this mechanism were:

1. The reaction is initiated by fluorene being adsorbed on the catalyst forming a reactive species.
2. The adsorbed fluorene species is attacked by decalin in the gas phase and undergoes hydrogenation by hydrogen transfer from decalin. This is suggesting that an Eley-Rideal type mechanism is responsible for the interactions between decalin, fluorene, and the catalyst in the initial steps.
3. Partially hydrogenation fluorene then cracks by three routes: central ring cracking of both the phenyl-phenyl and methyl-phenyl bonds to produce benzenes, cracking of only the phenyl-methyl bond producing biphenyls, and side ring cracking forming indanes.
4. In addition to the gas phase attack of fluorene by decalin, three other mechanisms are operative; isomerization, cracking, and dehydrogenation.
5. The bifunctional catalyst has acidic sites promoting cracking by carbonium ion mechanisms and isomerization, and nickel metal sites responsible for hydrogenation and dehydrogenation.
6. Molecular hydrogen serves to control coke formation by "healing" the rupture of C-C bonds and keeps the catalyst sites relatively "clean" for hydrocarbons to react.

2) Recommendations

The reaction of fluorene and decalin on Ni-Y zeolite in hydrogen was found to be quite complex with twenty reaction pathways developed in the final model, and is not completely understood at this time. The following points are therefore recommended for future study:

1. The nature of coke formation and its influence on deactivation should be investigated so that deactivation may be incorporated into a kinetic model.
2. Pseudo-homogeneous rate expressions were found adequate to describe the interactions of the compound groups, however, if adsorption/desorption phenomena can be determined, Langmuir-Hinshelwood-Hougen-Watson type kinetics should be used.
3. Other model coal derived liquid compounds, such as phenanthrene, acenaphthene, or anthracene should be studied in the same type of reactor system to see if they react in a similar scheme to that of fluorene on a Ni-Y zeolite.
4. Other catalysts should be evaluated for hydrocracking coal derived liquids. A metal loaded type L zeolite would be suitable for this work as it contains slightly larger pores than the Y type used in this study.
5. Finally, model compound work should be extended to the refining of either synthetic or actual coal liquids. A study which has been proposed relative to this is the extraction and refining of the heavy components found in tar sands. A concentrated extract of ten to twenty weight percent in decalin should be adequate for analytical purposes using the present reactor system.

NOMENCLATURE

A - frequency factor of equation 4.4, s^{-1} or m^3/kg-mole·s

a - coke coefficient of equation 4.6

C_c - weight % coke on catalyst

C - concentration, kg-mole/m^3

D_{eff} - effective diffusivity, m^2/s

E - apparent activation energy, kcal/kg-mole

F - minimization function

k - rate coefficient, 1/s or $m^3 \cdot kg\text{-}mole^{-1} s^{-1}$

K_k - rate coefficient of HJB solution method matrix, same units as k

M - molecular weight

n - exponent of Voorhies equation 4.6

R - gas constant, 1.987 kcal/kg-mole°K

R_{ij} - concentration function term of matrix equation 5.1, $(kg\text{-}mole/m^3)^d$ where d is order of reaction

Rp - catalyst particle radius, m

Rr - pore radius, m

r_A - rate of reaction of species A, kg-mole/m^3 s

T - temperature, °K

t - space time, s

V - volume of catalyst, m^3

W_{ij} - weighting factor of minimization, $kg\text{-}mole^{-1}$ m^3

X_{ijk} - integral of R_{jk} with space-time

Y_{ij} - measured change in concentration, kg-mole/m^3

$\hat{Y}_{ij}$ - predicted change in concentration, kg-mole/m^3

Matrix Terms

G - constant vector

K - solution vector

S - coefficient matrix

Subscripts

A - denotes activation energy

i - time interval step

j - compound group number

k - rate coefficient number

L - rate coefficient number in matrix operations

M - total number of compound groups in model

N - total number of rate coefficients in model

P - total number of time interval steps in integration

Greek Letters

ε - porosity of catalyst

η - effectiveness factor = observed reaction rate/reaction rate without diffusion limitations

λ - tortuosity of catalyst

τ - catalyst exposure time, s

Φ - modified Thiele modulus defined by equation 4.1

HYDROCRACKING OF MODEL COAL DERIVED LIQUID COMPONENTS OVER A ZEOLITE CATALYST

VOLUME II

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

in

The Department of Chemical Engineering

by
William David Constant
B.S., Louisiana State University, 1977
M.S., Louisiana State University, 1980
August, 1984

APPENDICES

APPENDIX 1

Gas Chromatograph Calibration Data

Gas Chromatograph Calibration

1) Introduction

The majority of the liquid and gas product analyses were performed on the Perkin-Elmer GC after the components of the liquid samples were identified with the GC/MS. The identity of the components of the gas samples were found on a Carle Analytical GC using external standards. After product identification was made, all composition determinations were made using the Perkin-Elmer GC and a H.P. integrator. Due to lack of field control of numeric output in the BASIC language used for the material balance program employing the results of the G.C. analysis, more digits are expressed in the data of Appendix 3 than are significant. Based on the analytical technqiues employed, no more than four significant figures should be used in analysis of the material balance data.

2) Liquid Sample Analysis

The thermal conductivity response curve for each component of the liquid sample injected into the GC was integrated by the H.P. integrator to yield a given number of area "counts" for each species. These area "counts" were converted to weight percent for the material balance calculations by the H.P. integrator using the relationship:

$$\text{weight \% component "j"} = \frac{RF(j) \times A(j)}{\sum_{j} RF(j)\ A(j)} \times 100 \qquad \text{A1.1}$$

where: $RF(j)$ = weight response factor

$A(j)$ = area "counts" under response curve.

This is a normalization procedure which is relatively insensitive to the sample injection size. Therefore to calculate the weight percent of each compound in the mixture, a value of RF relative to a reference compound with units of weight amount/area must be provided.

If a known composition sample is injected, and an area "count" determined, then the RF or more commonly determined RMR (relative molar response) value is known. The RMR is defind as:

$$RMR"j" = \frac{A(j)/n(j)}{(A_\phi/n_\phi)RMR_\phi} \qquad A1.2$$

where: $A(j)$ = area "counts" of species j

$n(j)$ = moles of j

A_ϕ = area "counts" of reference (benzene)

n_ϕ = moles of reference (benzene)

RMR_ϕ = 100

Therefore, the RMR value is a ratio of area to moles for the compound of interest and will adjust the detector response for each compound to mole percent by a normalization calculation similar to equation A1.1 using:

$$\text{Molar } RF(j) = RMR_\phi/RMR_j \qquad A1.3$$

Many of the RMR values needed were obtained from Carson et al. (1973) and Barry and Rosie (1971). Those which were not available from the literature were calculated by the method used by Barry and Rosie or were estimated from RMR values of compounds with similar structure and molecular weight. The calculation method uses the following equation:

$$RMR_j = \left\{ \frac{\frac{\sigma_j + \sigma_1}{\sigma_1}}{\frac{\sigma_\phi + \sigma_1}{\sigma_1}} \right\}^2 \times \left\{ \frac{M_j - M_1}{M_\phi - M_1} \right\}^{1/4} \times 100 \qquad A1.4$$

where: σ = molecular collision diameter, $\mathring{A}$

M = molecular weight

j = component of interest

1 = carrier gas, He

ϕ = standard (benzene)

Molecular collision diameters may be estimated by one of several empirical expressions reported in the literature. these are summarized by Barry and Rosie with the following used in this study:

$$\sigma = 2.3647\ (T_c/P_c)^{1/3} \qquad \text{A1.5}$$

where: T_c = critical temperature, °K

P_c = critical pressure, atm.

The molecular contribution method of Hougen, Watson, and Ragatz (1943) was used when needed for estimation of critical temperature and pressure to obtain σ. Values for the RMR of each compound were determined by one or more of the above methods and then converted to weight response factors by first dividing each RMR into the reference RMR (benzene = 100) by equation A1.3. For weight % then, each ratio of RMR was multiplied by its respective molecular weight and subsequently normalized by the molecular weight of benzene:

$$RF(j) = \frac{100}{RMR_j} \times \frac{M_j}{M_\phi} \qquad \text{A1.6}$$

which will reference each RF to benzene (RF = 1.0). These values of RF are listed in Table A1.1 with the compound identification number, initial RMR, retention time, and molecular weight.

The values of RMR for the analytical systems of this study were checked by making a standard of as many of the compounds in the samples as could be obtained in the laboratory. The mole fractions of the standard by G.C. analysis were found to be in agreement with the known

Table A1.1 Liquid Sample Analysis Reference Data

No.	Compound	RMR	RF	Retention time/min	MW
1	isobutane	91.75b	0.81106	2.66	58.13
2	n-butane	91.75b	0.81106	2.82	58.13
3	2-methyl butane	106.31b	0.8687	3.39	72.15
4	2-methyl pentane	120 a	0.9192	4.87	86.18
5	3-methyl pentane	119 a	0.9270	5.27	86.18
6	methylcyclopentane	115 a	0.9369	6.74	84.16
7	benzene	100 a	1.0000	7.86	78.12
8	cyclohexane	110 a	0.9794	8.19	84.16
9	dimethylcyclopentane	122.78b	1.0238	9.65	98.19
10	methylcyclohexane	120 a	1.0474	12.34	98.19
11	ethylcyclopentane	126 a	0.9976	13.18	98.19
12,13	trimethylcyclopentane	134.6 c	1.0672	13.73;14.37	112.22
14	toluene	115 a	1.0258	14.65	92.15
15,17	dimethylcyclohexane	134.6 c	1.0672	15.66;16.72	112.22
16,18	methylethylcyclopentane	134.6 c	1.0672	16.15;17.74	112.22
19,20,21	xylene	130 a	1.0454	18.37;18.62;19.27	106.17
22,24,26,28	mesitylene	150 a	1.0257	20.73;21.63;22.15;22.84	120.19
23,25,27	dimethyloctahydropentalene	153.8 c	1.1507	21.44;21.85;22.44	138.25
29	trans-decalin	159.24 b	1.1114	23.32	138.25
30	cis-decalin	159.24 b	1.1114	24.07	138.25
31,32	methyl indan	150.43 b	1.1251	24.31;24.50	132.21
33	tetralin	150 b	1.1251	24.69	132.21
34	naphthalene	139.35 b	1.1775	25.07	128.19
35,36,37,38	dimethyl indan	159.7 c	1.1720	25.55;24.77;26.09;26.39	146.21
39,40	methylnaphthalene	155.1 a,b	1.1735	26.98;27.32	142.20
41	biphenyl	165.1 a,b	1.1957	28.54	154.21
42	ethylene bis-benzene	176.9 b,c	1.2174	29.01	168.24
43,44,45	dimethylnaphthalene	167.3 b	1.1953	29.36;29.74;30.30	156.23
46,47	methylbiphenyl	176.9 b,c	1.2174	31.20;31.52	168.24

Table A1.1 Continued

No.	Compound	RMR		RF	Retention time/min	MW
48	fluorene	179.5	a,b	1.1854	35.60	166.23
49	methyl biphenyl	176.9	b,c	1.2174	36.19	168.24
50	methyl fluorene	167.8	b	1.3747	40.94	180.25
51	1-ethenyl-2-methylbenzene	145	c	1.0417	22.65	118
52	butylbenzene	148	c	1.1590	23.03	134
53	1-ethenyl-4-ethylbenzene	150	c	1.1230	23.64	132

RMR subscripts:
- a - Literature or Experimental Values
- b - Calculated
- c - Estimated from similar compounds by molecular weight

Compounds 51,52,53: observed only during tetralin feedstock runs

composition. A second standard of benzene, toluene, xylenes, and decalins was prepared and used to back calculate the RMR values from G.C. analysis of area "counts". The results were:

Compound	Literature RMR	Exp. RMR
benzene	100	100
toluene	116	115
xylene	127	130
decalin	153	159

The close agreement between RMR values shows that the literature and calculated RMR values are in close agreement for the analytical systems used.

3) Gas Sample Analysis

The hydrogen content of the gas samples could not be directly measured by the thermal conductivity detector with helium as a carrier gas due to the highly nonlinear negative response curve.

After identification of each compound was made using known standards, isobutane was found to be one of the primary products. A standard was prepared of 1.0685 mole % isobutane in helium and was analyzed for area "counts" with the Perkin-Elmer G.C. Area counts for a 1.0×10^{-6} m^3 (1 cc) injection size were calculated by the H.P. integrator as:

Sample no.	Area counts
1	318880
2	345280
3	325750
4	344660

giving an average area of 333643 counts for the isobutane standard. The total number of moles contained in the 1.0×10^{-6} m^3 (1 cc) injection sample size was calculated by the ideal gas law for room temperature and barometric pressure at the time of analysis. Therefore, the actual

number of moles/unit area count for the standard can be obtained as:

$$\left(\frac{\text{moles isobutane}}{\text{unit area}} \right)_{STD} = n_T \ (0.010685)/(333643) \qquad \text{A1.7}$$

where: n_T = total moles in 1 cc for a given room temperature and barometric pressure.

For a run sample, the moles of isobutane calculated as:

$$\left(\begin{matrix}\text{moles isobutane} \\ \text{in sample}\end{matrix} \right) = \left(\frac{\text{moles isobutane}}{\text{unit area}} \right)_{STD} \times \left(\begin{matrix}\text{area counts of} \\ \text{isobutane}\end{matrix} \right) \qquad \text{A1.8}$$

The moles of the other gases in the run sample were then determined using the ratio of RMR values, i.e., the area to mole conversion was adjusted for thermal conductivity response of the various gases from isobutane. As an example:

$$\left(\begin{matrix}\text{moles propane} \\ \text{in sample}\end{matrix} \right) = \left(\frac{\text{moles isobutane}}{\text{unit area}} \right) \times \left(\begin{matrix}\text{area counts} \\ \text{of propane}\end{matrix} \right) \times \frac{1.370}{1.149} \qquad \text{A1.9}$$

This calculation on each component of the gas yields the total moles of hydrocarbon in the 1 cc gas sample and with n_T known, the remainder is hydrogen. Thus the complete composition of the product gas was determined and converted from moles to mole fractions for the material balance calculations.

Table A1.2 lists the hydrocarbon components of the product gas with their identification numbers, retention times, and RMR values referenced to benzene (1.0). Methane concentration could not be resolved by the analytical system, however, samples were checked on the Carle Analytical GC and shown to be negligible in the reaction products.

Table A1.2

Gas Sample Analysis Reference Data

No.	Compound	$\frac{100}{RMR}$	Ret. time/min
3	ethane	1.724	0.78
4	propane	1.370	1.53
5	isobutane	1.149	2.90
6	n-butane	1.149	3.63
7	2-methylbutane	0.941	7.12

APPENDIX 2

Sample Material Balance Calculations

Sample Calculations

1) Introduction

The material balance calculations were performed by program MATBALSICONC listed in Appendix 4. Calculations are straight forward but repetitive in nature hence the example below using Run 82 data is given in a descriptive outline form. Run data was stored by program DATASTORE under a user supplied file name. The following calculations were then performed by the material balance routine.

The feedstock densities were adjusted to the feed pump temperature and then using the feed composition, molecular weights, and carbon and hydrogen numbers, the feedrates and total kg-atoms of carbon and hydrogen fed were determined. The hydrogen feedrate was calculated by the ideal gas law and then feed ratios, space velocity, and space time were determined. The last step before actual material balance work was to determine the kg·moles/s of product gas at the wet test meter (WTM).

The first material balance step calculated the mole fraction composition of the product gas based on the isobutane standard. The molecular weights, carbon numbers, and hydrogen numbers were then read from dataset MATBALDATA for each product from condenser A(1-53) and condenser B(54-106). With this data, product weights, and weight % GC product analysis, the kg·moles/s of each were calculated with the total kg-atoms of carbon and hydrogen summed and compared to the feedstock as a check of material balance closure. Products were grouped by their respective parent structures and two distributions were calculated. Finally, feedstock conversions were determined.

2) Sample Calculation

i) Run 82 Data:

Catalyst: NH_4 Y/5 % Ni

Weight: 7.0023×10^{-3} kg

Volume: 1.3×10^{-5} m^3

Feedstock: 20 wt % fluorene in decalin

Pump temperature: 383.7°K

Barometric pressure: 1.020 bar

Pressure correction: 4.368×10^{-3} bar

H_2O vapor pressure: 3.89×10^{-2} bar

at 301.5°K

H_2 feedrate: 78 s/rev at 300.1°K

where one revolution = 1.416×10^{-3} m^3

Material Balance Data:

Initial Pump volume: 6.545×10^{-5} m^3

Initial time: 8536.2 s

Final Pump volume: 7.598×10^{-5} m^3

Final time: 12243.6 s

WTM gas volume during MB: 0.06797 m^3

at 301.5°K

Reactor pressure: 15.15 bar

Reactor temperature: 660.9°K

Room temperature: 297.0°K

Liquid Sample weight: 8.4215×10^{-3} kg

(Cond A+B), total sample weight during material balance period.

ii) Analytical Data:

Gas sample injection volume = 7.0×10^{-8} m^3

GC area counts:

Gas 2	=	0
Gas 3	=	806
Gas 4	=	4806
Gas 5	=	8272
Gas 6	=	1991
Gas 7	=	1577

Wt % Product Distribution

COMP#	WT%	COMP#	WT%
1	.13	27	2.46
2	.069	28	3.456
3	.203	29	33.164
4	.344	30	7.896
5	.11	31	2.556
6	3.188	32	3.98
7	.534	33	.996
8	0	34	2.892
9	1	35	.048
10	.828	36	1.39
11	.182	37	.196
12	.017	38	.379
13	0	39	1.156
14	1.306	40	.577
15	.107	41	1.493
16	.071	42	1.075
17	.083	43	1.181
18	.13	44	.069
19	.254	45	0
20	.716	46	.721
21	.488	47	.444
22	1.586	48	8.754
23	3.958	49	2.159
24	1.416	50	2.681
25	1.616	51	0
26	3.191	52	0
		53	0

Wt% Distribution of Feedstock

trans-decalin	=	30.28%
cir-decalin	=	46.31%
tetralin	=	1.01%
fluorene	=	22.40%

iii) Calculations

Adjust density of feedstock components to pump temperature[1]:

$$\frac{\rho_2}{\rho_1} = \left(\frac{T_c - T_2}{T_c - T_1} \right)^{0.29} \qquad \text{A2.1}$$

where: ρ = density, kg/m^3

T_c = critical temperature, °K

1 = reference conditions of density

2 = pump temperature or component density

0.29 = exponent for hydrocarbons.

yields for each component at 383.7°K:

component	density/kg/m^3
trans-decalin	812.1
cis-decalin	832.3
tetralin	898.7
fluorene	1091.0

Calculate the liquid feedstock rate in terms of kg, kg-mole, and kg-atoms of C and H:

$$FR = \frac{7.598 \times 10^{-5} - 6.545 \times 10^{-5}}{12243.6 - 8536.2} \qquad \text{A2.2}$$

$$FR = 2.840 \times 10^{-9} \ m^3/s$$

Convert the wt% of the feedstock components to volume % as for trans-decalin:

$$V\% \text{ trans-decalin} = \frac{\left(\frac{30.28}{812.1} \right) \times 100}{\left(\frac{30.28}{812.1} \right) + \left(\frac{46.31}{832.3} \right) + \left(\frac{1.01}{898.7} \right) + \left(\frac{22.40}{1091.0} \right)}$$

$$V\% = 32.54\% \qquad \text{A2.3}$$

Therefore, the flowrate of trans-decalin is:

$$FR_{TD} = (2.84 \times 10^{-9})(0.3254) = 9.241 \times 10^{-10} \ m^3/s$$

or:

$$FR_{TD} = 7.501 \times 10^{-7} \ kg/s = 5.425 \times 10^{-9} \ kg\text{-mole/s}$$

[1]Perry, R.H. and C.H. Chilton, ed.; Chemical Engineer's Handbook, 5th ed., p. 3-230, McGraw-Hill, New York (1973).

which is composed of:

5.425×10^{-8} kg-atoms C/s

and

9.765×10^{-8} kg-atoms H/s

Repeating this and summing for each quantity yields:

Total kg-mole/s = 1.725×10^{-8}

Total kg/s fed = 2.477×10^{-6}

Total kg-atoms C/s = 1.825×10^{-7}

Total kg-atoms H/s = 2.828×10^{-7}

The hydrogen feedrate during the run is:

$$N = \frac{(1.020 - 4.368 \times 10^{-3} - 0.0389 \text{ bars})(1.416 \times 10^{-3} \frac{m^3}{rev})}{(78 \text{ sec/rev})(300.1°K)(0.08314 \frac{m^3 \cdot bar}{kg\text{-mole} \cdot °K})}$$

$N = 7.108 \times 10^{-7}$ kg-mole H_2/s A2.4

$$H_2\text{/hydrocarbon molar ratio} = \frac{7.108 \times 10^{-7}}{1.725 \times 10^{-8}} = 41.2$$

$$\text{WHSV, liquid feed basis} = \frac{2.477 \times 10^{-6} \text{ kg/s}}{7.0023 \times 10^{-3} \text{ kg}} = 3.54 \times 10^{-4} \text{s} \quad \text{A2.5}$$

$$\text{VHSV, liquid feed basis} = \frac{2.84 \times 10^{-9} \text{ m}^3\text{/s}}{1.3 \times 10^{-5} \text{ m}^3} = 2.19 \times 10^{-4} \text{s} \quad \text{A2.6}$$

WHSV, total feed basis =

$$\frac{(7.108 \times 10^{-7} \text{kg-mole } H_2\text{/s})(2 \text{ kg/kg-mole}) + 2.477 \times 10^{-6} \text{kg/s}}{7.0023 \times 10^{-3} \text{ kg catalyst}} \quad \text{A2.7}$$

WHSV = 5.56×10^{-4} s

Molar Gas Density:

$$MGD = (15.15 \text{ bar})/(0.08314 \frac{m^3 \cdot bar}{kg \cdot mole °K})(660.9°K) \quad \text{A2.8}$$

MGD = 0.2757 kg-mole/m^3

Space time:

$$ST = \frac{(0.2757 \frac{\text{kg-mole}}{m^3})(1.3 \times 10^{-5} m^3 \text{ cat. vol.})}{(7.108 \times 10^{-7} \text{ kg-mole } H_2/s)+(1.725 \times 10^{-8} \text{ kg·mole FS/s})}$$

$$ST = 4.92 \text{ s} \qquad \text{A2.9}$$

Superficial Gas Velocity:

$$SGV = (1.3 \times 10^{-5} \text{ m}^3 \text{ cat.})/(1.96 \times 10^{-4} \text{ m}^2)(4.92 \text{ s}) \qquad \text{A2.10}$$

$$SGV = 1.35 \times 10^{-2} \text{ m/s}$$

where 1.96×10^{-4} m^3 = CSA of reactor.

From the WTM reading at the end of the M.B. period, the product gas rate is:

$$NM = \frac{(0.97967 \text{ bar}) (\frac{0.6797 \text{ m}^3 \text{ gas}}{3707.4 \text{ s}})}{(0.08314 \frac{\text{m}^3\text{·bar}}{\text{kg-mole·K}})(301.48°K)} \qquad \text{A2.11}$$

$$NM = 7.145 \times 10^{-7} \text{ kg-mole/s}$$

Gas composition based on G.C. analysis:

Kg-moles in G.C. sample:

$$TT = \frac{(1.0158 \text{ bar})(7.0 \times 10^{-8} \text{ m}^3)}{(0.08314 \text{ m}^3\text{·bar/kg·mole·°K})(297.0°K)} \qquad \text{A2.12}$$

$$TT = 2.879 \times 10^{-9} \text{ kg-moles}$$

Kg-moles/area count for isobutane standard:

$$CN_{ISOB} = \frac{(2.879 \times 10^{-9} \text{ kg-moles})(0.010685)}{(333643 \text{ counts}/1.0 \times 10^{-6} \text{ m}^3)(7.0 \times 10^{-8} \text{ m}^3)}$$

$$CN_{ISOB} = 1.317 \times 10^{-15} \text{ kg-mole/count} \qquad \text{A2.13}$$

Ratio the mole/count of all other compounds by RMR values as for propane (4):

$$CN_{PROP} = (1.317 \times 10^{-15})(1.37)/(1.149) = 1.570 \times 10^{-15} \frac{\text{kg-mole}}{\text{count}}$$

A2.14

Kg-moles of each compound in gas sample:

$$GS_{ETH} = (2.79 \times 10^{-15})(806) = 2.253 \times 10^{-12}$$

$$GS_{PROP} = (1.570 \times 10^{-15})(4806) = 7.545 \times 10^{-12}$$

$$GS_{ISOB} = (1.317 \times 10^{-15})(8272) = 1.089 \times 10^{-11}$$

$$GS_{NBUT} = (1.317 \times 10^{-15})(1991) = 2.622 \times 10^{-12}$$

$$GS_{2MB} = (1.078 \times 10^{-15})(1517) = 1.635 \times 10^{-12}$$

$$2.495 \times 10^{-11}$$

Fraction of gas that is hydrocarbon:

$$Y = (2.495 \times 10^{-11})/(2.879 \times 10^{-9}) = 8.66 \times 10^{-3} \qquad \text{A2.15}$$

H_2 fraction = 0.99134

Product distribution at WTM as for isobutane:

$MGAS_{ISOB}$ = (kg-mole/s product gas)(H_2 free mole fraction isobutane)(mole fraction hydrocarbon) A2.16

$$MGAS_{ISOB} = (7.145 \times 10^{-7})(2.622 \times 10^{-12}/2.495 \times 10^{-11})(8.66 \times 10^{-3})$$

$$MGAS_{ISOB} = 6.506 \times 10^{-10} \text{ kg-mole/s}$$

$$\text{kg-atoms C} = (4)(6.506 \times 10^{-10}) = 2.602 \times 10^{-9} \text{ kg-atoms/s}$$

$$\text{kg-atoms H} = (10)(6.506 \times 10^{-14}) = 6.506 \times 10^{-9} \text{ kg-atoms/s}$$

For all components of the gas by the same procedure:

Component	kg-mole/s	kg-atoms C/s	kg-atoms H/s
ethane	5.92×10^{-10}	1.118×10^{-9}	3.355×10^{-9}
propane	1.873×10^{-9}	5.619×10^{-9}	1.498×10^{-8}
isobutane	2.704×10^{-9}	1.082×10^{-8}	2.704×10^{-8}
n-butane	6.508×10^{-10}	2.603×10^{-9}	6.508×10^{-9}
2-methylbutane	4.219×10^{-10}	2.109×10^{-9}	5.063×10^{-9}
hydrogen	7.083×10^{-7}	0.0	1.4116×10^{-6}
Σ	7.145×10^{-7}	2.227×10^{-8}	1.474×10^{-6}

For the liquid product analysis, calcualte the kg-moles, kg-atoms of C and H, and sum for the balance check as for component 29 (trans-decalin); with a GC analysis of 33.164 wt% of product sample.

$$GM_{29} = \frac{(0.33164)(8.4215 \times 10^{-3}\text{kg}/(12243.6 - 8536.2\ \text{s})}{138.25\ \text{kg/kg-mole}} \quad \text{A2.17}$$

$$GH_{29} = 5.449 \times 10^{-9}\ \text{kg-mole/s}$$

$$C_{29} = (10)(GM_{29}) = 5.449 \times 10^{-8}\ \text{kg-atoms C/s}$$

$$H_{29} = (18)(GM_{29}) = 9.809 \times 10^{-8}\ \text{kg-atoms H/s}$$

Repeat this calculation for each component in condenser A (and B if not included in A) and sum:

Total liquid kg-mole/s = 1.709×10^{-8}

Total liquid kg-atoms C/s = 1.686×10^{-7}

Total liquid kg-atoms H/s = 2.468×10^{-7}

Carbon balance:

C_{in} = 1.825×10^{-7} kg-atoms/s

C_{out} = $2.227 \times 10^{-8} + 1.686 \times 10^{-7}$ kg-atoms/s

C_{BAL} = $(1.909/1.825) \times 100 = 104.6\%$ A2.18

Hydrogen balance:

H_{in} = $(7.108 \times 10^{-7}$ kg·mole H_2/s)(2 kg-atoms H/kg-mole H_2) + 2.828×10^{-7} kg atoms H/s

H_{out} = $1.474 \times 10^{-6} + 2.468 \times 10^{-7}$ kg-atom H/s

H_{BAL} = $H_{out}/H_{in} = (1.721/1.704)(100) = 101.0\%$ A2.19

The final set of calculations for the MB determines two product groupings; by concentration at reaction conditions and as feedstock free mole fractions. The individual compounds are grouped by GC identification numbers (1-53) according to the list in Table A2.1. For trans-decalin (Group 7):

Total kg-mole/s product = $7.145 \times 10^{-7} + 1.709 \times 10^{-8}$

= 7.316×10^{-7} kg-mole/s

Mole fraction trans-decalin = $\frac{5.449 \times 10^{-9}}{7.316 \times 10^{-7}} = 7.448 \times 10^{-3}$ A2.20

Table A2.1

Compound Grouping Scheme

Group Number/Name	G.C. identification Numbers
1/Alkanes	All gases + 1 thru 5
2/Cyclopentanes	6, 9, 11, 12, 13, 16, 18
3/Cyclohexanes	8, 10, 15, 17
4/Benzenes	7, 14, 19, 20, 21, 22, 24, 26, 28
5/Alkylbenzenes	51, 52, 53
6/Dimethyloctahydropentalene	23, 25, 27
7/trans-decalin	29
8/cis-decalin	30
9/tetralin	33
10/Indanes	31, 32, 35 thru 38
11/Naphthalenes	34, 39, 40, 43, 44, 45
12/Biphenyls	41, 42, 46, 47, 49
13/Fluorene	48
14/Methylfluorene	50

Concentration of trans-decalin:

$$CI_{29} = (MGD)(7.448 \times 10^{-3}) = 2.0534 \times 10^{-3} \text{ kg-mole/m}^3 \quad \text{A2.21}$$

where MGD = 0.2757 kg-mole/m^3

Repeating this for each compound group yields the concentration product distribution of Table A2.2. Removing the feedstock compounds (Groups 7,8,9,13) and calculation of mole fractions yields the second list of Table A2.2.

Conversion was defined as:

$$\% \text{ conv.} = \frac{(\text{kg-mole/s fed}) - (\text{kg-mole/s product})}{(\text{kg-mole/s fed})} \times 100. \quad \text{A2.22}$$

For fluorene:

$$\% \text{ conv.} = \frac{(3.337 \times 10^{-9}) - \frac{(0.08754)(2.2717 \times 10^{-6} \text{kg/s})}{(166.23 \text{ kg/kg-mole})}}{3.337 \times 10^{-9}} \times 100$$

$$\% \text{ conv.} = 64.15\% \quad \text{A2.23}$$

Conversion of the other components of the feedstock was calculated by the same method.

Table A2.2

Run 82 Product Distribution

With Feedstock		Without Feedstock	
Compound Group	Conc./kg-mole/m^3	Compound Group	Mole Fraction
1	2.376×10^{-3}	1	0.4197
2	4.439×10^{-4}	2	0.0784
3	8.668×10^{-5}	3	0.0153
4	9.846×10^{-4}	4	0.1739
5	0.0	5	0.0
6	4.974×10^{-4}	6	0.0879
7	2.053×10^{-3}	7	0.0
8	4.889×10^{-4}	8	0.0
9	6.449×10^{-5}	9	0.0
10	4.678×10^{-4}	10	0.0826
11	2.704×10^{-4}	11	0.0654
12	2.067×10^{-4}	12	0.0542
13	4.508×10^{-4}	13	0.0
14	1.273×10^{-4}	14	0.0225
H_2	0.2699		

APPENDIX 3

Experimental Run and Material Balance Data

Experimental Run and Material Balance Data

The following data is paired by run number, with the first page being the input data for the material balance calculations and the second page consisting of the material balance calculations results. Data covers run 62 to run 124 excluding run 67, for which no balance was made. Notation is consistent with the S.I. system except for the total kg-atoms of C and H in the feedstock which is on a per hour basis. Due to the lack of field control of numeric output in the BASIC language used for the material balance output programs, more digits are expressed in the numbers than are significant. Based on analytical techniques employed, no more than four significant figures should be taken in analysis of the data.

RUN NUMBER =62 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN62TET
PUMP TEMP/ DEG K =379.261111
INITIAL TIME OF M. B./S =8627.4 FINAL TIME=12240
INITIAL PUMP VOL/M3= 1.1868E-04 FINAL VOL/M3= 1.2894E-04
WT % OF TRANS-DECALIN =0
CIS-DECALIN = 0
TETRALIN = 81
FLUORENE = 19
BAROMETRIC PRESSURE/ BARS =1.0147842
P CORRECTION/ BARS = 4.70654E-03
H20 VAPOR PRESS/ BARS = .036490922
WTM SEC/REV AVERAGE=76.2 WTM TEMP/K=299.816667
KGMS OF CATALYST =6.9234E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.1480392 REACTOR TEMP/K=660.594445
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.372223
KGS/SEC IN COND A=2.27470974E-06 KGS/SEC IN B = 4.111E-08
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =5E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =76
GC AREA COUNTS, GAS 4 =1430 GAS 5 =1168
GC AREA COUNTS, GAS 6 =1310 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	8E-03	27	0	1	.025	27	0
2	.015	28	0	2	4E-03	28	0
3	0	29	.373	3	.333	29	2.703
4	0	30	.214	4	1.74	30	4.412
5	0	31	.291	5	.66	31	.154
6	.133	32	0	6	11.58	32	0
7	.898	33	28.55	7	4.428	33	17.384
8	0	34	33.915	8	1.307	34	2.449
9	.174	35	.602	9	9.912	35	.076
10	.233	36	.446	10	8.377	36	0
11	.054	37	0	11	2.072	37	0
12	0	38	0	12	.296	38	0
13	0	39	1.893	13	.075	39	.219
14	.516	40	.759	14	12.266	40	.147
15	0	41	1.162	15	.835	41	0
16	0	42	.854	16	.527	42	0
17	0	43	.568	17	.328	43	0
18	.012	44	0	18	.311	44	0
19	0	45	.091	19	5.062	45	0
20	.612	46	.755	20	2.976	46	0
21	.114	47	.419	21	1.027	47	0
22	.307	48	5.443	22	1.081	48	0
23	.346	49	2.141	23	.553	49	0
24	.162	50	1.064	24	.338	50	0
25	.354	51	1.962	25	.326	51	1.344
26	.2	52	3.408	26	0	52	1.978
		53	10.955			53	2.697

RUN NUMBER 62 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	0	0
C-DECALIN	0	0
TETRALIN	1.62409506E-08	2.14721608E-06
FLUORENE	3.02994628E-09	5.0366797E-07

TOTAL KG-MOLE FED/S = 1.92708969E-08
TOTAL KGS FED/S = 2.65088405E-06
PUMP RATE/ M3/S = 2.8400825E-09
TOTAL KG-ATOMS CARBON= 7.26469897E-04
TOTAL KG-ATOMS HYDROGEN= 8.10680648E-04

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 37.6494505
WHSV (1/S) LIQ FEED BASIS= 3.82884543E-04
VHSV (1/S) = 2.18466138E-04
TOTAL WHSV (1/S) = 5.92473149E-04
MOLAR GAS DENSITY =.275749511 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.81300514
SUPERFICIAL GAS VELOCITY/ M/S = .0137806898

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.27454597E-06 KGS/S,COND B= 4.111144E-08
KG-MOLE/S OF ALL GAS OUT= 7.33218471E-07
H2 FEEDRATE KG-MOLE/S = 7.2553868E-07
FRACTION OF GAS THAT IS HYDROCARBONS =2.75222199E-03
KG-MOLE/S FREE H2 IN GAS= 7.31200491E-07
H BALANCE CLOSURE = 99.2945 C BALANCE CLOSURE=91.5081967

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	7.49457343E-04	1	.147159775
	2	7.43259372E-05	2	.0145942772
	3	3.66157622E-05	3	7.18969182E-03
	4	2.89769528E-04	4	.056897726
	5	1.0517309E-03	5	.206512731
	6	4.32591601E-05	6	8.4941569E-03
	7	2.54915976E-05	7	5.00540532E-03
	8	1.77502209E-05	8	3.48534647E-03
	9	1.8238695E-03	9	0
	10	7.85221717E-05	10	.0154182292
	11	2.40661377E-03	11	.472550899
	12	2.69964095E-04	12	.0530088282
	13	2.73544095E-04	13	0
	14	4.93133799E-05	14	9.68293387E-03
	H2	.268559284		

KG-MOLE FLUORENE/S IN PRODUCT = 7.44772528E-10
FLUORENE CONVERSION = 75.4196128 %
T-DECALIN CONVERSION= 0 %
C-DECALIN CONVERSION= 0 %

RUN NUMBER =63 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN63TET
PUMP TEMP/ DEG K =380.927778
INITIAL TIME OF M. B./S =8835 FINAL TIME=12451.8
INITIAL PUMP VOL/M3= 1.5683E-04 FINAL VOL/M3= 1.6709E-04
WT % OF TRANS-DECALIN =0
CIS-DECALIN = 0
TETRALIN = 81
FLUORENE = 19
BAROMETRIC PRESSURE/ BARS =1.0198632
P CORRECTION/ BARS = 5.28216E-03
H20 VAPOR PRESS/ BARS = .036490922
WTM SEC/REV AVERAGE=77.7 WTM TEMP/K=299.261111
KGMS OF CATALYST =3.8144E-03 VOLUME/M3=7.3E-06
REACTOR PRESS/BARS=15.4927892 REACTOR TEMP/K=659.816667
INITIAL WTM M3 = 0 FINAL M3 = .066552
WTM TEMP/DEG K DURING M.B.=300.372223
KGS/SEC IN COND A=2.48194854E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =6E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =66
GC AREA COUNTS, GAS 4 =706 GAS 5 =673
GC AREA COUNTS, GAS 6 =703 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	9E-03	27	0	1	0	27	0
2	9E-03	28	0	2	0	28	0
3	0	29	.376	3	0	29	0
4	6E-03	30	.19	4	0	30	0
5	0	31	0	5	0	31	0
6	.062	32	0	6	0	32	0
7	.418	33	43.73	7	0	33	0
8	0	34	27.194	8	0	34	0
9	.074	35	.379	9	0	35	0
10	.099	36	.241	10	0	36	0
11	.02	37	0	11	0	37	0
12	0	38	0	12	0	38	0
13	0	39	.752	13	0	39	0
14	.161	40	.283	14	0	40	0
15	0	41	.998	15	0	41	0
16	0	42	.536	16	0	42	0
17	0	43	.383	17	0	43	0
18	0	44	0	18	0	44	0
19	0	45	.137	19	0	45	0
20	.373	46	.58	20	0	46	0
21	0	47	.253	21	0	47	0
22	.177	48	10.912	22	0	48	0
23	.068	49	1.769	23	0	49	0
24	0	50	1.122	24	0	50	0
25	.167	51	.738	25	0	51	0
26	0	52	1.375	26	0	52	0
		53	6.412			53	0

RUN NUMBER 63 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	0	0
C-DECALIN	0	0
TETRALIN	1.61946969E-08	2.14110088E-06
FLUORENE	3.02131709E-09	5.02233539E-07

TOTAL KG-MOLE FED/S = 1.9216014E-08
TOTAL KGS FED/S = 2.64333441E-06
PUMP RATE/ M3/S = 2.83678446E-09
TOTAL KG-ATOMS CARBON= 7.24400933E-04
TOTAL KG-ATOMS HYDROGEN= 8.08371854E-04

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 37.268373
WHSV (1/S) LIQ FEED BASIS= 6.92982716E-04
VHSV (1/S) = 3.88597503E-04
TOTAL WHSV (1/S) = 1.0684776E-03
MOLAR GAS DENSITY =.282357456 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =2.80299479
SUPERFICIAL GAS VELOCITY/ M/S = .0132875374

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.48176985E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.20426404E-07
H2 FEEDRATE KG-MOLE/S = 7.16149576E-07
FRACTION OF GAS THAT IS HYDROCARBONS =1.23658032E-03
KG-MOLE/S FREE H2 IN GAS= 7.19535539E-07
H BALANCE CLOSURE = 99.1677582 C BALANCE CLOSURE=96.1251752

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	3.44064554E-04	1	.095349708
	2	1.60673164E-05	2	4.45269329E-03
	3	9.56297099E-06	3	2.65016109E-03
	4	1.14611521E-04	4	.0317619903
	5	6.17372255E-04	5	.171090755
	6	1.61223233E-05	6	4.46793721E-03
	7	2.57957173E-05	7	7.14869953E-03
	8	1.30350699E-05	8	3.61237476E-03
	9	3.13718461E-03	9	0
	10	4.02197639E-05	10	.0111459978
	11	2.11426727E-03	11	.585921346
	12	2.38290717E-04	12	.0660368819
	13	6.22615397E-04	13	0
	14	5.90394751E-05	14	.016361455
	H2	.274989207		

KG-MOLE FLUORENE/S IN PRODUCT = 1.62913269E-09
FLUORENE CONVERSION = 46.0787253 %
T-DECALIN CONVERSION= 0 %
C-DECALIN CONVERSION= 0 %

RUN NUMBER =64 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN64FL
PUMP TEMP/ DEG K =370.372222
INITIAL TIME OF M. B./S =8490 FINAL TIME=11972.4
INITIAL PUMP VOL/M3= 3.244E-05 FINAL VOL/M3= 4.234E-05
WT % OF TRANS-DECALIN =38.69
CIS-DECALIN = 59.63
TETRALIN = 1.68
FLUORENE = 0
BAROMETRIC PRESSURE/ BARS =1.0161386
P CORRECTION/ BARS = 4.26636E-03
H20 VAPOR PRESS/ BARS = .03714442
WTM SEC/REV AVERAGE=78.75 WTM TEMP/K=299.816667
KGMS OF CATALYST =7.0078E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.1480392 REACTOR TEMP/K=660.5
INITIAL WTM M3 = 0 FINAL M3 = .065136
WTM TEMP/DEG K DURING M.B.=300.65
KGS/SEC IN COND A=0 KGS/SEC IN B = 9.4404774E-07
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =5944
GC AREA COUNTS, GAS 4 =22572 GAS 5 =27967
GC AREA COUNTS, GAS 6 =5357 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	0	27	0	1	10.889	27	.104
2	0	28	0	2	6.438	28	.125
3	0	29	0	3	19.493	29	3.362
4	0	30	0	4	9.43	30	4.791
5	0	31	0	5	3.79	31	0
6	0	32	0	6	9.06	32	0
7	0	33	0	7	7.533	33	1.447
8	0	34	0	8	1.559	34	.361
9	0	35	0	9	1.134	35	0
10	0	36	0	10	.787	36	0
11	0	37	0	11	.21	37	0
12	0	38	0	12	0	38	0
13	0	39	0	13	0	39	0
14	0	40	0	14	14.117	40	0
15	0	41	0	15	0	41	0
16	0	42	0	16	.025	42	0
17	0	43	0	17	0	43	0
18	0	44	0	18	0	44	0
19	0	45	0	19	.199	45	0
20	0	46	0	20	3.51	46	0
21	0	47	0	21	.899	47	0
22	0	48	0	22	.104	48	0
23	0	49	0	23	.26	49	0
24	0	50	0	24	0	50	0
25	0	51	0	25	0	51	0
26	0	52	0	26	.059	52	0
		53	0			53	.315

RUN NUMBER 64 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	6.64086314E-09	9.18099328E-07
C-DECALIN	1.02350651E-08	1.41499775E-06
TETRALIN	3.01533742E-10	3.9865776E-08
FLUORENE	0	0

TOTAL KG-MOLE FED/S = 1.7177462E-08
TOTAL KGS FED/S = 2.37296286E-06
PUMP RATE/ M3/S = 2.84288973E-09
TOTAL KG-ATOMS CARBON= 6.18383685E-04
TOTAL KG-ATOMS HYDROGEN= 1.10657756E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 40.918028
WHSV (1/S) LIQ FEED BASIS= 3.38614668E-04
VHSV (1/S) = 2.18682076E-04
TOTAL WHSV (1/S) = 5.39208934E-04
MOLAR GAS DENSITY =.275784291 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.97916493
SUPERFICIAL GAS VELOCITY/ M/S = .0133208141

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 0 KGS/S,COND B= 9.43979774E-07
KG-MOLE/S OF ALL GAS OUT= 7.29119528E-07
H2 FEEDRATE KG-MOLE/S = 7.02867871E-07
FRACTION OF GAS THAT IS HYDROCARBONS =.0316382678
KG-MOLE/S FREE H2 IN GAS= 7.06051449E-07
H BALANCE CLOSURE = 101.728326 C BALANCE CLOSURE=84.4382428

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	.0111230112	1	.875201517
2	4.27169773E-04	2	.0336113689
3	9.32588684E-05	3	7.33796825E-03
4	1.03811246E-03	4	.0816827012
5	8.38565708E-06	5	6.59815913E-04
6	9.25202333E-06	6	7.27984959E-04
7	8.54541276E-05	7	0
8	1.21775944E-04	8	0
9	3.84595945E-05	9	0
10	0	10	0
11	9.89585971E-06	11	7.78644493E-04
12	0	12	0
13	0	13	0
14	0	14	0
H2	.262829516		

KG-MOLE FLUORENE/S IN PRODUCT = 0
FLUORENE CONVERSION = 0 %
T-DECALIN CONVERSION= 96.5432281 %
C-DECALIN CONVERSION= 96.8038062 %

RUN NUMBER =65.1 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN65ASV
PUMP TEMP/ DEG K =372.594445
INITIAL TIME OF M. B./S =3669 FINAL TIME=7260.6
INITIAL PUMP VOL/M3= 6.495E-05 FINAL VOL/M3= 8.536E-05
WT % OF TRANS-DECALIN =38.69
CIS-DECALIN = 59.63
TETRALIN = 1.68
FLUORENE = 0
BAROMETRIC PRESSURE/ BARS =1.0218948
P CORRECTION/ BARS = 4.36794E-03
H20 VAPOR PRESS/ BARS = .03037242
WTM SEC/REV AVERAGE=38.7 WTM TEMP/K=296.761111
KGMS OF CATALYST =7.0078E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.1480392 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .13452
WTM TEMP/DEG K DURING M.B.=297.316667
KGS/SEC IN COND A=5.0190126E-07 KGS/SEC IN B = 1.308E-06
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =3443
GC AREA COUNTS, GAS 4 =15830 GAS 5 =25498
GC AREA COUNTS, GAS 6 =5616 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.456	27	.036	1	9.654	27	.022
2	.209	28	.324	2	5.724	28	.021
3	.74	29	7.045	3	18.783	29	.741
4	.945	30	12.73	4	9.039	30	1.394
5	.451	31	0	5	3.576	31	0
6	4.759	32	0	6	19.36	32	0
7	1.634	33	1.594	7	5.653	33	.425
8	.665	34	.38	8	2.199	34	.103
9	1.55	35	0	9	2.5	35	0
10	1.362	36	.084	10	1.482	36	0
11	.45	37	0	11	.421	37	0
12	.065	38	.043	12	.055	38	0
13	.019	39	.156	13	.024	39	0
14	17.252	40	.121	14	13.435	40	0
15	.285	41	.185	15	.122	41	0
16	.258	42	0	16	.097	42	0
17	.119	43	.047	17	.037	43	0
18	.013	44	0	18	.029	44	0
19	1.225	45	0	19	.205	45	0
20	22.935	46	0	20	3.65	46	0
21	6.995	47	0	21	.874	47	0
22	1.998	48	.558	22	0	48	0
23	3.471	49	0	23	0	49	0
24	.338	50	0	24	.264	50	0
25	7.524	51	0	25	0	51	0
26	.981	52	0	26	.033	52	0
		53	0			53	0

RUN NUMBER 65.1 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	1.32487399E-08	1.83163829E-06
C-DECALIN	2.04192908E-08	2.82296695E-06
TETRALIN	6.0156971E-10	7.95335313E-08
FLUORENE	0	0

TOTAL KG-MOLE FED/S = 3.42696003E-08
TOTAL KGS FED/S = 4.73413877E-06
PUMP RATE/ M3/S = 5.68274954E-09
TOTAL KG-ATOMS CARBON= 1.23369574E-03
TOTAL KG-ATOMS HYDROGEN= 2.20765854E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.7023761
WHSV (1/S) LIQ FEED BASIS= 6.75547375E-04
VHSV (1/S) = 4.37131084E-04
TOTAL WHSV (1/S) = 1.09319105E-03
MOLAR GAS DENSITY =.275610478 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =2.39237062
SUPERFICIAL GAS VELOCITY/ M/S = .027724187

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 5.01865126E-07 KGS/S,COND B= 1.30801046E-06
KG-MOLE/S OF ALL GAS OUT= 1.49518841E-06
H2 FEEDRATE KG-MOLE/S = 1.46339336E-06
FRACTION OF GAS THAT IS HYDROCARBONS =.0252328677
KG-MOLE/S FREE H2 IN GAS= 1.45746052E-06
H BALANCE CLOSURE = 98.5949349 C BALANCE CLOSURE=76.3225

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	8.48812203E-03	1	.807736933
2	6.95038369E-04	2	.0661404441
3	1.24519873E-04	3	.0118494174
4	1.11604471E-03	4	.106203767
5	0	5	0
6	7.31644203E-05	6	6.96238865E-03
7	5.92282961E-05	7	0
8	1.07969522E-04	8	0
9	1.8640936E-05	9	0
10	7.92364922E-07	10	7.5402122E-05
11	6.68461379E-06	11	6.36113551E-04
12	1.0943539E-06	12	1.0413965E-04
13	3.06212836E-06	13	2.91394747E-04
14	0	14	0
H2	.264916116		

KG-MOLE FLUORENE/S IN PRODUCT = 1.68465825E-11
FLUORENE CONVERSION = 0 %
T-DECALIN CONVERSION= 97.5405212 %
C-DECALIN CONVERSION= 97.0909651 %

RUN NUMBER =65.2 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN65BSV
PUMP TEMP/ DEG K =377.038889
INITIAL TIME OF M. B./S =2157 FINAL TIME=3998.1
INITIAL PUMP VOL/M3= 1.2145E-04 FINAL VOL/M3= 1.4236E-04
WT % OF TRANS-DECALIN =38.69
CIS-DECALIN = 59.63
TETRALIN = 1.68
FLUORENE = 0
BAROMETRIC PRESSURE/ BARS =1.0161386
P CORRECTION/ BARS = 4.43566E-03
H20 VAPOR PRESS/ BARS = .030924338
WTM SEC/REV AVERAGE=19.44 WTM TEMP/K=297.872223
KGMS OF CATALYST =7.0078E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.1480392 REACTOR TEMP/K=660.65
INITIAL WTM M3 = 0 FINAL M3 = .1416
WTM TEMP/DEG K DURING M.B.=297.594445
KGS/SEC IN COND A=3.39954972E-06 KGS/SEC IN B = 1.537E-06
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =1020
GC AREA COUNTS, GAS 4 =9151 GAS 5 =19699
GC AREA COUNTS, GAS 6 =3833 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.326	27	2.345	1	3.99	27	.167
2	.116	28	0	2	2.37	28	0
3	.315	29	8.022	3	9.69	29	.372
4	.435	30	4.855	4	6.09	30	.528
5	.19	31	0	5	2.373	31	.176
6	4.53	32	3.643	6	32.541	32	0
7	.43	33	7.324	7	3.083	33	.216
8	.4	34	3.259	8	2.209	34	.135
9	1.715	35	0	9	5.879	35	0
10	1.739	36	.178	10	3.957	36	0
11	.429	37	.624	11	.978	37	.047
12	.104	38	1.412	12	.185	38	0
13	.037	39	.546	13	.078	39	.027
14	5.111	40	1.984	14	11.526	40	0
15	.425	41	0	15	.438	41	0
16	.28	42	0	16	.298	42	0
17	.056	43	.455	17	.143	43	0
18	.014	44	.61	18	.148	44	0
19	1.585	45	.219	19	1.11	45	0
20	8.09	46	0	20	7.034	46	0
21	4.008	47	0	21	2.036	47	0
22	1.679	48	.147	22	.053	48	0
23	3.643	49	0	23	.161	49	0
24	2.829	50	0	24	0	50	0
25	9.116	51	3.522	25	1.3	51	.148
26	1.11	52	8.257	26	0	52	.344
		53	3.896			53	.169

RUN NUMBER 65.2 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	2.63743576E-08	3.64625494E-06
C-DECALIN	4.06488225E-08	5.61969972E-06
TETRALIN	1.19754896E-09	1.58327948E-07
FLUORENE	0	0

TOTAL KG-MOLE FED/S = 6.82207291E-08
TOTAL KGS FED/S = 9.42428259E-06
PUMP RATE/ M3/S = 1.13574316E-08
TOTAL KG-ATOMS CARBON= 2.4559266E-03
TOTAL KG-ATOMS HYDROGEN= 4.39480103E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.2691282
WHSV (1/S) LIQ FEED BASIS= 1.34481681E-03
VHSV (1/S) = 8.73641595E-04
TOTAL WHSV (1/S) = 2.16778769E-03
MOLAR GAS DENSITY =.275726329 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =1.21431277
SUPERFICIAL GAS VELOCITY/ M/S = .0546206316

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 3.39930497E-06 KGS/S,COND B= 1.53687341E-06
KG-MOLE/S OF ALL GAS OUT= 3.04763861E-06
H2 FEEDRATE KG-MOLE/S = 2.88363075E-06
FRACTION OF GAS THAT IS HYDROCARBONS =.0164576661
KG-MOLE/S FREE H2 IN GAS= 2.99748159E-06
H BALANCE CLOSURE = 100.611098 C BALANCE CLOSURE=79.7706895

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	4.99638641E-03	1	.6139976
	2	8.74821062E-04	2	.107505302
	3	1.7926983E-04	3	.0220301706
	4	1.07400758E-03	4	.131983002
	5	3.73486893E-04	5	.0458971819
	6	3.47091316E-04	6	.0426534734
	7	1.79465601E-04	7	0
	8	1.116149E-04	8	0
	9	1.70054889E-04	9	0
	10	1.31609379E-04	10	.0161732573
	11	1.58117558E-04	11	.0194308032
	12	0	12	0
	13	2.67892466E-06	13	3.29208587E-04
	14	0	14	0
	H2	.267127725		

KG-MOLE FLUORENE/S IN PRODUCT = 3.00606287E-11
FLUORENE CONVERSION = 0 %
T-DECALIN CONVERSION= 92.3645105 %
C-DECALIN CONVERSION= 96.9188577 %

RUN NUMBER =66 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN66TP
PUMP TEMP/ DEG K =372.594445
INITIAL TIME OF M. B./S =9265.2 FINAL TIME=13246.2
INITIAL PUMP VOL/M3= 8.46E-05 FINAL VOL/M3= 9.592E-05
WT % OF TRANS-DECALIN =30.943
CIS-DECALIN = 47.613
TETRALIN = 1.127
FLUORENE = 30.317
BAROMETRIC PRESSURE/ BARS =1.0103824
P CORRECTION/ BARS = 4.13092E-03
H20 VAPOR PRESS/ BARS = .030924338
WTM SEC/REV AVERAGE=78.9 WTM TEMP/K=298.15
KGMS OF CATALYST =7.0078E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.4927892 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .073632
WTM TEMP/DEG K DURING M.B.=298.844445
KGS/SEC IN COND A=1.30963254E-06 KGS/SEC IN B =4.335E-07
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =722
GC AREA COUNTS, GAS 4 =7488 GAS 5 =9798
GC AREA COUNTS, GAS 6 =3445 GAS 7 =745

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.127	27	3.168	1	.997	27	.116
2	.074	28	3.995	2	1.047	28	.27
3	.113	29	29.435	3	5.795	29	.176
4	.164	30	3.332	4	5.239	30	.152
5	.066	31	4.01	5	2.013	31	.262
6	1.746	32	6.804	6	27.192	32	.12
7	.794	33	1.21	7	8.324	33	0
8	0	34	3.8	8	2.233	34	.102
9	.829	35	.475	9	6.815	35	0
10	.878	36	.952	10	4.612	36	0
11	.231	37	.159	11	1.162	37	0
12	.04	38	1.085	12	.188	38	0
13	0	39	2.09	13	.075	39	0
14	3.794	40	1.007	14	23.333	40	0
15	.17	41	.369	15	.431	41	0
16	.109	42	.474	16	.296	42	0
17	.085	43	.502	17	.147	43	0
18	.128	44	.757	18	.127	44	0
19	1.169	45	.164	19	.777	45	0
20	5.88	46	.307	20	5.866	46	0
21	2.345	47	.19	21	1.276	47	0
22	2.01	48	.295	22	0	48	0
23	3.328	49	.349	23	.065	49	0
24	1.995	50	.222	24	.259	50	0
25	3.969	51	0	25	0	51	0
26	4.807	52	0	26	.047	52	0
		53	0			53	0

RUN NUMBER 66 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.17018413E-09	7.14777956E-07
C-DECALIN	7.9555304E-09	1.09985208E-06
TETRALIN	1.96910259E-10	2.60335054E-08
FLUORENE	4.2129427E-09	7.00317465E-07

TOTAL KG-MOLE FED/S = 1.75355675E-08
TOTAL KGS FED/S = 2.540981E-06
PUMP RATE/ M3/S = 2.8435294E-09
TOTAL KG-ATOMS CARBON= 6.76774797E-04
TOTAL KG-ATOMS HYDROGEN= 1.01071068E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 40.2544455
WHSV (1/S) LIQ FEED BASIS= 3.62590353E-04
VHSV (1/S) = 2.18731282E-04
TOTAL WHSV (1/S) = 5.6404556E-04
MOLAR GAS DENSITY =.281882906 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =5.06553111
SUPERFICIAL GAS VELOCITY/ M/S = .0130936972

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.30953825E-06 KGS/S,COND B= 4.3347569E-07
KG-MOLE/S OF ALL GAS OUT= 7.25791854E-07
H2 FEEDRATE KG-MOLE/S = 7.05884546E-07
FRACTION OF GAS THAT IS HYDROCARBONS =.0109177829
KG-MOLE/S FREE H2 IN GAS= 7.17867816E-07
H BALANCE CLOSURE = 100.697031 C BALANCE CLOSURE=83.3652689

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	3.38130613E-03	1	.444473848
2	8.46107073E-04	2	.111221064
3	1.85530936E-04	3	.0243881051
4	1.95113254E-03	4	.25647704
5	0	5	0
6	3.79182274E-04	6	.0498436397
7	1.06255702E-03	7	0
8	1.21855022E-04	8	0
9	4.55843423E-05	9	0
10	5.03149121E-04	10	.0661391242
11	3.03896251E-04	11	.0399472662
12	5.09967666E-05	12	6.70354243E-03
13	8.83908356E-06	13	0
14	6.13440337E-06	14	8.06369423E-04
H2	.273036635		

KG-MOLE FLUORENE/S IN PRODUCT = 2.32397151E-11
FLUORENE CONVERSION = 99.4483734 %
T-DECALIN CONVERSION= 45.9656669 %
C-DECALIN CONVERSION= 95.9728496 %

RUN NUMBER =68 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN68TP
PUMP TEMP/ DEG K =390.372222
INITIAL TIME OF M. B./S =8628.6 FINAL TIME=12195.6
INITIAL PUMP VOL/M3= 1.6217E-04 FINAL VOL/M3= 1.723E-04
WT % OF TRANS-DECALIN =30.94
CIS-DECALIN = 47.61
TETRALIN = 1.13
FLUORENE = 20.32
BAROMETRIC PRESSURE/ BARS =1.0158
P CORRECTION/ BARS = 4.43566E-03
H20 VAPOR PRESS/ BARS = .04290062
WTM SEC/REV AVERAGE=78.3 WTM TEMP/K=302.594445
KGMS OF CATALYST =7.003E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.2859392 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .065136
WTM TEMP/DEG K DURING M.B.=303.15
KGS/SEC IN COND A=1.32685614E-06 KGS/SEC IN B =4.323E-07
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =5E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =1141
GC AREA COUNTS, GAS 4 =7948 GAS 5 =12084
GC AREA COUNTS, GAS 6 =3180 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.144	27	2.824	1	1.087	27	.101
2	.066	28	4.006	2	.906	28	0
3	.125	29	33.213	3	5.62	29	1.293
4	.19	30	3.858	4	4.964	30	.173
5	.072	31	4.071	5	1.756	31	.305
6	2.212	32	6.724	6	34.023	32	0
7	.477	33	1.362	7	6.167	33	.186
8	0	34	4.426	8	2.207	34	0
9	1.018	35	.172	9	7.485	35	0
10	1.049	36	.451	10	5.143	36	0
11	.275	37	.726	11	1.276	37	0
12	.038	38	.926	12	.187	38	0
13	0	39	2.247	13	.078	39	0
14	2.603	40	.949	14	16.749	40	0
15	.163	41	.603	15	.44	41	0
16	.109	42	.485	16	.297	42	0
17	.086	43	.411	17	.152	43	0
18	.172	44	.705	18	.144	44	0
19	.868	45	.181	19	1.056	45	0
20	3.133	46	.559	20	5.556	46	0
21	1.606	47	.364	21	1.356	47	0
22	1.833	48	1.27	22	0	48	0
23	2.788	49	.822	23	0	49	0
24	1.525	50	.707	24	.156	50	0
25	3.679	51	0	25	.39	51	0
26	3.711	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 68 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.47772212E-09	7.57295083E-07
C-DECALIN	8.42903523E-09	1.16531412E-06
TETRALIN	2.09198692E-10	2.76581591E-08
FLUORENE	2.99198303E-09	4.9735734E-07

TOTAL KG-MOLE FED/S = 1.71079391E-08
TOTAL KGS FED/S = 2.4476247E-06
PUMP RATE/ M3/S = 2.83994423E-09
TOTAL KG-ATOMS CARBON= 6.48194038E-04
TOTAL KG-ATOMS HYDROGEN= 1.01789851E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 40.6782302
WHSV (1/S) LIQ FEED BASIS= 3.49508085E-04
VHSV (1/S) = 2.18455501E-04
TOTAL WHSV (1/S) = 5.48255798E-04
MOLAR GAS DENSITY =.278119449 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =5.07073861
SUPERFICIAL GAS VELOCITY/ M/S = .0130802504

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.32676061E-06 KGS/S,COND B= 4.3222568E-07
KG-MOLE/S OF ALL GAS OUT= 7.01423138E-07
H2 FEEDRATE KG-MOLE/S = 6.95920683E-07
FRACTION OF GAS THAT IS HYDROCARBONS =.0169426582
KG-MOLE/S FREE H2 IN GAS= 6.89539166E-07
H BALANCE CLOSURE = 100.756035 C BALANCE CLOSURE=95.0223227

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	4.97410272E-03	1	.550958678
	2	1.05610053E-03	2	.116979441
	3	2.07127723E-04	3	.0229425935
	4	1.48861984E-03	4	.164887632
	5	0	5	0
	6	3.51987601E-04	6	.0389880616
	7	1.25265967E-03	7	0
	8	1.45784821E-04	8	0
	9	5.54030285E-05	9	0
	10	5.04397998E-04	10	.0558698663
	11	3.37172515E-04	11	.037347062
	12	8.83819916E-05	12	9.78967021E-03
	13	3.93378933E-05	13	0
	14	2.01957935E-05	14	2.23699596E-03
	H2	.267598177		

KG-MOLE FLUORENE/S IN PRODUCT = 1.01364734E-10
FLUORENE CONVERSION = 96.612122 %
T-DECALIN CONVERSION= 41.0737386 %
C-DECALIN CONVERSION= 95.5433326 %

RUN NUMBER =69 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN69FL
PUMP TEMP/ DEG K =377.038889
INITIAL TIME OF M. B./S =9558.6 FINAL TIME=13240.8
INITIAL PUMP VOL/M3= 3.533E-05 FINAL VOL/M3= 4.579E-05
WT % OF TRANS-DECALIN =36.925
CIS-DECALIN = 56.732
TETRALIN = 1.231
FLUORENE = 5.112
BAROMETRIC PRESSURE/ BARS =1.014107
P CORRECTION/ BARS = 4.60496E-03
H20 VAPOR PRESS/ BARS = .04415344
WTM SEC/REV AVERAGE=77.88 WTM TEMP/K=302.594445
KGMS OF CATALYST =7.003E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.1480392 REACTOR TEMP/K=661.483334
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=303.705556
KGS/SEC IN COND A=1.43947626E-06 KGS/SEC IN B = 3.328 E-07
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =865
GC AREA COUNTS, GAS 4 =6856 GAS 5 =11537
GC AREA COUNTS, GAS 6 =2594 GAS 7 =1420

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.136	27	3.108	1	1.092	27	0
2	.048	28	0	2	.704	28	0
3	.101	29	44.109	3	3.516	29	1.203
4	.151	30	6.598	4	4.594	30	.325
5	.057	31	4.084	5	1.573	31	0
6	1.79	32	7.955	6	37.84	32	.176
7	.189	33	0	7	3.708	33	.312
8	.205	34	3.753	8	2.574	34	0
9	.75	35	.266	9	9.744	35	0
10	.801	36	.58	10	7.15	36	0
11	.204	37	.679	11	1.622	37	0
12	.033	38	0	12	.215	38	0
13	0	39	1.709	13	.05	39	0
14	1.499	40	.607	14	12.617	40	0
15	.12	41	.127	15	.596	41	0
16	.077	42	.287	16	.377	42	0
17	.07	43	.387	17	.236	43	0
18	.157	44	.573	18	.256	44	0
19	.439	45	.112	19	1.24	45	0
20	1.819	46	.171	20	5.115	46	0
21	1.037	47	.133	21	1.471	47	0
22	1.812	48	.432	22	.133	48	0
23	4.256	49	.334	23	0	49	0
24	3.046	50	.328	24	.278	50	0
25	1.684	51	0	25	.478	51	.196
26	3.187	52	0	26	.077	52	.315
		53	0			53	.219

```
RUN NUMBER  69   MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES
COMPOUND          KG-MOLE/SECOND          KG/S
T-DECALIN      6.37364956E-09          8.81157052E-07
C-DECALIN      9.79254941E-09          1.35381996E-06
TETRALIN      2.22191052E-10          2.93758789E-08
FLUORENE      7.33861759E-10          1.2198984E-07
TOTAL KG-MOLE FED/S =  1.71222518E-08
TOTAL   KGS FED/S =  2.38634273E-06
PUMP RATE/ M3/S  =  2.84071579E-09
TOTAL KG-ATOMS CARBON=   6.24321777E-04
TOTAL KG-ATOMS HYDROGEN=   1.0835787E-03


FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 40.7319779
WHSV (1/S) LIQ FEED BASIS=  3.40757338E-04
VHSV (1/S) =        2.18514851E-04
TOTAL WHSV (1/S) = 5.39934148E-04
MOLAR GAS DENSITY =.275379067  KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC    =5.01011741
SUPERFICIAL GAS VELOCITY/  M/S   =    .0132385182


MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.43937263E-06  KGS/S,COND B= 3.32808218E-07
KG-MOLE/S  OF ALL GAS OUT= 7.05448575E-07
H2 FEEDRATE KG-MOLE/S  = 6.97423181E-07
FRACTION OF GAS THAT IS HYDROCARBONS =.011330295
KG-MOLE/S FREE H2 IN GAS=  6.97455635E-07
H BALANCE CLOSURE = 98.9842822  C BALANCE CLOSURE=91.5842708
                    PRODUCT DISTRIBUTION
          WITH FEEDSTOCK                WITHOUT FEEDSTOCK
COMPOUND GROUP CONC./KG-MOLE/M3   COMP. GROUP   MOLE FRAC.
       1       3.28696852E-03         1       .494220552
       2       9.1325638E-04          2       .137314997
       3       2.08636623E-04         3       .0313700926
       4       9.75629209E-04         4       .146693223
       5       7.21628381E-06         5       1.08502279E-03
       6       3.64589855E-04         6       .0548188393
       7       1.76699977E-03         7       0
       8       2.65649984E-04         8       0
       9       3.0030006E-06          9       0
       10      5.60250448E-04         10      .084237888
       11      2.89459335E-04         11      .0435223981
       12      3.47916313E-05         12      5.23118463E-03
       13      1.43027211E-05         13      0
       14      1.00148142E-05         14      1.50580299E-03
       H2      .266678298
KG-MOLE FLUORENE/S  IN PRODUCT =  3.74065436E-11
FLUORENE CONVERSION =  94.9027806  %
T-DECALIN CONVERSION=  27.4934527  %
C-DECALIN CONVERSION=  92.9051546  %
```

RUN NUMBER =70 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN70FL
PUMP TEMP/ DEG K =378.15
INITIAL TIME OF M. B./S =8142.6 FINAL TIME=11905.2
INITIAL PUMP VOL/M3= 3.938E-05 FINAL VOL/M3= 5.008E-05
WT % OF TRANS-DECALIN =34.5
CIS-DECALIN = 54.74
TETRALIN = 1.23
FLUORENE = 9.53
BAROMETRIC PRESSURE/ BARS =1.0137684
P CORRECTION/ BARS = 4.43566E-03
H20 VAPOR PRESS/ BARS = .04144464
WTM SEC/REV AVERAGE=76.98 WTM TEMP/K=302.316667
KGMS OF CATALYST =7.003E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.1480392 REACTOR TEMP/K=660.372223
INITIAL WTM M3 = 0 FINAL M3 = .069384
WTM TEMP/DEG K DURING M.B.=302.316667
KGS/SEC IN COND A=1.88217834E-06 KGS/SEC IN B = 1.74 4E-07
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =343
GC AREA COUNTS, GAS 4 =4165 GAS 5 =7112
GC AREA COUNTS, GAS 6 =1999 GAS 7 =1489

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.07	27	1.971	1	.366	27	1.4
2	.028	28	0	2	.286	28	0
3	.047	29	46.374	3	1.899	29	5.626
4	.078	30	18.133	4	3.115	30	1.306
5	.028	31	2.754	5	1.077	31	.693
6	1.002	32	5.7	6	33.287	32	0
7	.023	33	0	7	3.987	33	0
8	.122	34	2.944	8	3.023	34	.405
9	.435	35	.046	9	9.796	35	0
10	.442	36	.127	10	7.626	36	0
11	.104	37	.225	11	1.748	37	0
12	0	38	.343	12	0	38	0
13	0	39	1.094	13	0	39	0
14	.77	40	.408	14	13.317	40	0
15	.062	41	.245	15	.575	41	0
16	.041	42	.273	16	.335	42	0
17	.052	43	.223	17	.201	43	0
18	.11	44	.378	18	.18	44	0
19	.214	45	.063	19	1.246	45	0
20	.817	46	.301	20	5.073	46	0
21	.473	47	.085	21	1.436	47	0
22	1.075	48	1.871	22	.491	48	0
23	2.975	49	.584	23	0	49	0
24	1.583	50	1.381	24	.785	50	0
25	1.325	51	0	25	0	51	0
26	2.602	52	0	26	.722	52	0
		53	0			53	0

RUN NUMBER 70 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	6.02289737E-09	8.32665561E-07
C-DECALIN	9.55633049E-09	1.32116269E-06
TETRALIN	2.24539274E-10	2.96863374E-08
FLUORENE	1.3836779E-09	2.30008777E-07

TOTAL KG-MOLE FED/S = 1.7187445E-08
TOTAL KGS FED/S = 2.41352337E-06
PUMP RATE/ M3/S = 2.84380098E-09
TOTAL KG-ATOMS CARBON= 6.33686673E-04
TOTAL KG-ATOMS HYDROGEN= 1.06903791E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.1976733
WHSV (1/S) LIQ FEED BASIS= 3.44638592E-04
VHSV (1/S) = 2.18752172E-04
TOTAL WHSV (1/S) = 5.46859663E-04
MOLAR GAS DENSITY =.275842278 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.94433433
SUPERFICIAL GAS VELOCITY/ M/S = .0134146532

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.88204283E-06 KGS/S,COND B= 1.74362506E-07
KG-MOLE/S OF ALL GAS OUT= 7.09855493E-07
H2 FEEDRATE KG-MOLE/S = 7.08082745E-07
FRACTION OF GAS THAT IS HYDROCARBONS =7.23330726E-03
KG-MOLE/S FREE H2 IN GAS= 7.0472089E-07
H BALANCE CLOSURE = 99.3737531 C BALANCE CLOSURE=96.4000825

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	2.03429192E-03	1	.449378771
2	4.77155865E-04	2	.105404595
3	1.29700713E-04	3	.0286511224
4	6.65319538E-04	4	.146970291
5	0	5	0
6	3.31198916E-04	6	.0731624405
7	2.42655311E-03	7	0
8	9.44537317E-04	8	0
9	0	9	0
10	4.97158488E-04	10	.109823211
11	2.73046498E-04	11	.060316466
12	6.42180985E-05	12	.0141858943
13	8.05175813E-05	13	0
14	5.48080995E-05	14	.0121072085
H2	.267863772		

KG-MOLE FLUORENE/S IN PRODUCT = 2.11833131E-10
FLUORENE CONVERSION = 84.6905749 %
T-DECALIN CONVERSION= -5.9955184 %
C-DECALIN CONVERSION= 73.9965408 %

RUN NUMBER =71 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN71FL
PUMP TEMP/ DEG K =374.816667
INITIAL TIME OF M. B./S =8076.6 FINAL TIME=11685.6
INITIAL PUMP VOL/M3= 4.156E-05 FINAL VOL/M3= 5.181E-05
WT % OF TRANS-DECALIN =32.8
CIS-DECALIN = 51.5
TETRALIN = 1.1
FLUORENE = 14.6
BAROMETRIC PRESSURE/ BARS =1.0188474
P CORRECTION/ BARS = 4.2325E-03
H20 VAPOR PRESS/ BARS = .03297964
WTM SEC/REV AVERAGE=78.6 WTM TEMP/K=298.427778
KGMS OF CATALYST =7.003E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.2859392 REACTOR TEMP/K=659.261111
INITIAL WTM M3 = 0 FINAL M3 = .065136
WTM TEMP/DEG K DURING M.B.=298.427778
KGS/SEC IN COND A=2.16220074E-06 KGS/SEC IN B = 1.198E-07
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =172
GC AREA COUNTS, GAS 4 =3046 GAS 5 =5792
GC AREA COUNTS, GAS 6 =1744 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.043	27	1.228	1	.175	27	.474
2	.02	28	0	2	.199	28	1.094
3	.028	29	42.16	3	1.645	29	10.945
4	.047	30	30.833	4	3.139	30	6.942
5	.016	31	1.436	5	1.069	31	0
6	.614	32	2.773	6	25.966	32	0
7	.035	33	.879	7	3.658	33	4.042
8	.18	34	2.251	8	2.328	34	6.384
9	.263	35	.034	9	6.502	35	0
10	.268	36	.081	10	4.598	36	0
11	.058	37	.083	11	.981	37	0
12	0	38	.163	12	.119	38	0
13	0	39	.69	13	0	39	0
14	.494	40	.261	14	8.717	40	0
15	.034	41	.355	15	.372	41	0
16	.024	42	.23	16	.233	42	0
17	.03	43	.113	17	.19	43	0
18	.076	44	.23	18	.202	44	0
19	.119	45	.048	19	.851	45	0
20	.441	46	.467	20	3.356	46	0
21	.213	47	0	21	1.059	47	0
22	.92	48	5.845	22	.604	48	0
23	1.752	49	.938	23	1.109	49	0
24	.838	50	0	24	1.234	50	0
25	.832	51	0	25	1.245	51	0
26	1.559	52	0	26	.568	52	0
		53	0			53	0

```
RUN NUMBER  71   MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES
COMPOUND          KG-MOLE/SECOND          KG/S
T-DECALIN      5.8098512E-09          8.03211929E-07
C-DECALIN      9.12217491E-09          1.26114068E-06
TETRALIN      2.03743933E-10          2.69369854E-08
FLUORENE      2.15079866E-09          3.57527261E-07
TOTAL KG-MOLE FED/S =  1.72865687E-08
TOTAL   KGS FED/S =  2.44861686E-06
PUMP RATE/ M3/S  =  2.84014463E-09
TOTAL KG-ATOMS CARBON=   6.45539935E-04
TOTAL KG-ATOMS HYDROGEN=   1.05381735E-03


FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.2168683
WHSV (1/S) LIQ FEED BASIS=  3.49678319E-04
VHSV (1/S) =        2.18470916E-04
TOTAL WHSV (1/S) = 5.53160405E-04
MOLAR GAS DENSITY =.278822362  KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC    =4.9668337
SUPERFICIAL GAS VELOCITY/  M/S   =   .0133538859


MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.16204507E-06  KGS/S,COND B= 1.19778736E-07
KG-MOLE/S  OF ALL GAS OUT= 7.13801215E-07
H2 FEEDRATE KG-MOLE/S  = 7.12498225E-07
FRACTION OF GAS THAT IS HYDROCARBONS =5.2272896E-03
KG-MOLE/S FREE H2 IN GAS=  7.10069969E-07
H BALANCE CLOSURE = 100.551673  C BALANCE CLOSURE=100.772402
                    PRODUCT DISTRIBUTION
          WITH FEEDSTOCK                 WITHOUT FEEDSTOCK
COMPOUND GROUP CONC./KG-MOLE/M3   COMP. GROUP   MOLE FRAC.
        1       1.4774587E-03          1       .471995041
        2       2.72583337E-04         2       .0870805952
        3       8.11926346E-05         3       .0259381334
        4       4.36238128E-04         4       .139362429
        5       0                      5       0
        6       2.36800684E-04         6       .0756493218
        7       2.55176054E-03         7       0
        8       1.86267472E-03         8       0
        9       6.88154908E-05         9       0
        10      2.82980979E-04         10      .0904022688
        11      2.43831624E-04         11      .0778954546
        12      9.9155915E-05          12      .0316767569
        13      2.90053345E-04         13      0
        14      0                      14      0
        H2      .270918816
KG-MOLE FLUORENE/S  IN PRODUCT =  7.60220986E-10
FLUORENE CONVERSION =  64.6540143  %
T-DECALIN CONVERSION=  -15.1163164  %
C-DECALIN CONVERSION=  46.4819106  %
```

RUN NUMBER =72 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN72TP
PUMP TEMP/ DEG K =381.483333
INITIAL TIME OF M. B./S =9894.6 FINAL TIME=13618.8
INITIAL PUMP VOL/M3= 7.832E-05 FINAL VOL/M3= 8.89E-05
WT % OF TRANS-DECALIN =30.993
CIS-DECALIN = 48.43
TETRALIN = 1.063
FLUORENE = 19.51
BAROMETRIC PRESSURE/ BARS =1.0218948
P CORRECTION/ BARS = 4.46952E-03
H20 VAPOR PRESS/ BARS = .04151236
WTM SEC/REV AVERAGE=73.8 WTM TEMP/K=302.316667
KGMS OF CATALYST =7.018E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.0101392 REACTOR TEMP/K=633.15
INITIAL WTM M3 = 0 FINAL M3 = .072216
WTM TEMP/DEG K DURING M.B.=302.872223
KGS/SEC IN COND A=1.43450364E-06 KGS/SEC IN B = 2.109E-07
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =370
GC AREA COUNTS, GAS 4 =3239 GAS 5 =5548
GC AREA COUNTS, GAS 6 =2783 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.072	27	4.18	1	.244	27	.369
2	.033	28	4.256	2	.236	28	0
3	.054	29	37.438	3	1.628	29	2.605
4	.071	30	7.545	4	3.656	30	1.38
5	.022	31	2.765	5	1.301	31	.131
6	1.042	32	4.553	6	34.445	32	0
7	.343	33	2.03	7	8.552	33	.121
8	0	34	2.724	8	0	34	0
9	.494	35	.118	9	9.529	35	0
10	.588	36	.321	10	7.958	36	0
11	.131	37	.288	11	1.703	37	0
12	0	38	.579	12	.427	38	0
13	0	39	1.058	13	.178	39	0
14	.791	40	.369	14	13.996	40	0
15	.107	41	.616	15	1.06	41	0
16	.059	42	.53	16	.543	42	0
17	.067	43	.266	17	.346	43	0
18	.125	44	.947	18	.332	44	0
19	.313	45	.039	19	1.373	45	0
20	.741	46	.603	20	5.109	46	0
21	.629	47	.264	21	1.338	47	0
22	2.395	48	2.554	22	.334	48	0
23	5.9	49	1.476	23	.444	49	0
24	2.44	50	1.465	24	0	50	0
25	2.095	51	0	25	.254	51	0
26	4.505	52	0	26	.2	52	.209
		53	0			53	0

RUN NUMBER 72 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.52586556E-09	7.63950914E-07
C-DECALIN	8.63477783E-09	1.19375803E-06
TETRALIN	1.98185008E-10	2.62020399E-08
FLUORENE	2.89300846E-09	4.80904795E-07

TOTAL KG-MOLE FED/S = 1.72518368E-08
TOTAL KGS FED/S = 2.46481578E-06
PUMP RATE/ M3/S = 2.8409013E-09
TOTAL KG-ATOMS CARBON= 6.52305399E-04
TOTAL KG-ATOMS HYDROGEN= 1.03031135E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 43.1674238
WHSV (1/S) LIQ FEED BASIS= 3.51210611E-04
VHSV (1/S) = 2.18529121E-04
TOTAL WHSV (1/S) = 5.63439564E-04
MOLAR GAS DENSITY =.285079643 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.86379903
SUPERFICIAL GAS VELOCITY/ M/S = .0136367745

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.43440036E-06 KGS/S,COND B= 2.10918354E-07
KG-MOLE/S OF ALL GAS OUT= 7.5125633E-07
H2 FEEDRATE KG-MOLE/S = 7.44717353E-07
FRACTION OF GAS THAT IS HYDROCARBONS =5.83219677E-03
KG-MOLE/S FREE H2 IN GAS= 7.46874856E-07
H BALANCE CLOSURE = 97.0269585 C BALANCE CLOSURE=75.6025992

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	1.72311908E-03	1	.375805438
	2	5.31397207E-04	2	.115895623
	3	1.13946629E-04	3	.0248513079
	4	1.02645231E-03	4	.223865177
	5	1.2269763E-06	5	2.67598664E-04
	6	4.77216409E-04	6	.104079006
	7	1.46358889E-03	7	0
	8	2.99826932E-04	8	0
	9	8.28652178E-05	9	0
	10	3.44694788E-04	10	.0751765661
	11	2.10869444E-04	11	.0459897895
	12	1.12730911E-04	12	.0245861646
	13	8.21981772E-05	13	0
	14	4.34823543E-05	14	9.48332901E-03
	H2	.278566028		

KG-MOLE FLUORENE/S IN PRODUCT = 2.2038492E-10
FLUORENE CONVERSION = 92.3821543 %
T-DECALIN CONVERSION= 28.9868994 %
C-DECALIN CONVERSION= 90.6902256 %

RUN NUMBER =73 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN73TP
PUMP TEMP/ DEG K =387.038889
INITIAL TIME OF M. B./S =8508 FINAL TIME=12144.6
INITIAL PUMP VOL/M3= 1.1472E-04 FINAL VOL/M3= 1.2505E-04
WT % OF TRANS-DECALIN =30.993
CIS-DECALIN = 48.43
TETRALIN = 1.063
FLUORENE = 19.51
BAROMETRIC PRESSURE/ BARS =1.0171544
P CORRECTION/ BARS = 4.43566E-03
H20 VAPOR PRESS/ BARS = .04151236
WTM SEC/REV AVERAGE=78 WTM TEMP/K=301.761111
KGMS OF CATALYST =7.0039E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.1480392 REACTOR TEMP/K=677.594445
INITIAL WTM M3 = 0 FINAL M3 = .066552
WTM TEMP/DEG K DURING M.B.=302.594445
KGS/SEC IN COND A=1.96368486E-06 KGS/SEC IN B =1.920E-07
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =363
GC AREA COUNTS, GAS 4 =4639 GAS 5 =7775
GC AREA COUNTS, GAS 6 =1655 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.014	27	2.355	1	.501	27	0
2	.083	28	2.926	2	.409	28	0
3	.043	29	36.382	3	2.783	29	2.552
4	.077	30	12.552	4	4.749	30	1.212
5	.026	31	2.897	5	1.577	31	0
6	.986	32	5.938	6	36.254	32	0
7	.293	33	0	7	6.497	33	0
8	0	34	4.19	8	2.478	34	0
9	.428	35	.192	9	8.697	35	0
10	.429	36	.146	10	5.86	36	0
11	.113	37	.234	11	1.456	37	0
12	0	38	0	12	.163	38	0
13	0	39	1.427	13	.036	39	0
14	.935	40	.606	14	15.981	40	0
15	.041	41	.565	15	.373	41	0
16	.028	42	.505	16	.259	42	0
17	.038	43	.22	17	.156	43	0
18	.062	44	.473	18	.135	44	0
19	.21	45	.058	19	.865	45	0
20	.795	46	.929	20	3.798	46	0
21	.414	47	.098	21	.888	47	0
22	1.114	48	7.621	22	0	48	0
23	2.934	49	1.546	23	0	49	0
24	1.533	50	3.943	24	.463	50	0
25	1.298	51	0	25	.397	51	0
26	2.305	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 73 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.49543493E-09	7.59743879E-07
C-DECALIN	8.58722659E-09	1.18718408E-06
TETRALIN	1.97093614E-10	2.60577467E-08
FLUORENE	2.87707682E-09	4.7825648E-07

TOTAL KG-MOLE FED/S = 1.7156832E-08
TOTAL KGS FED/S = 2.45124218E-06
PUMP RATE/ M3/S = 2.8405881E-09
TOTAL KG-ATOMS CARBON= 6.48713191E-04
TOTAL KG-ATOMS HYDROGEN= 1.02463748E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 40.9463251
WHSV (1/S) LIQ FEED BASIS= 3.49979665E-04
VHSV (1/S) = 2.18505029E-04
TOTAL WHSV (1/S) = 5.50583214E-04
MOLAR GAS DENSITY =.268833171 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.85622349
SUPERFICIAL GAS VELOCITY/ M/S = .0136580474

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.96354349E-06 KGS/S,COND B= 1.91973758E-07
KG-MOLE/S OF ALL GAS OUT= 7.06239494E-07
H2 FEEDRATE KG-MOLE/S = 7.02509219E-07
FRACTION OF GAS THAT IS HYDROCARBONS =7.09383269E-03
KG-MOLE/S FREE H2 IN GAS= 7.0122955E-07
H BALANCE CLOSURE = 99.8071511 C BALANCE CLOSURE=98.3219309

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	1.97988087E-03	1	.390686487
	2	5.16869377E-04	2	.101992945
	3	1.04056795E-04	3	.0205333484
	4	9.01133775E-04	4	.177819178
	5	0	5	0
	6	3.50030171E-04	6	.0690708515
	7	1.93517836E-03	7	0
	8	6.69360126E-04	8	0
	9	0	9	0
	10	5.16633077E-04	10	.101946316
	11	3.7894922E-04	11	.0747773978
	12	1.60378608E-04	12	.0316472348
	13	3.34837365E-04	13	0
	14	1.59765448E-04	14	.0315262411
	H2	.260826098		

KG-MOLE FLUORENE/S IN PRODUCT = 9.00208439E-10
FLUORENE CONVERSION = 68.7110044 %
T-DECALIN CONVERSION= 5.32657376 %
C-DECALIN CONVERSION= 79.0436289 %

RUN NUMBER =74 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN74TP
PUMP TEMP/ DEG K =384.261111
INITIAL TIME OF M. B./S =8671.8 FINAL TIME=12502.8
INITIAL PUMP VOL/M3= 1.5143E-04 FINAL VOL/M3= 1.6232E-04
WT % OF TRANS-DECALIN =30.993
CIS-DECALIN = 48.43
TETRALIN = 1.063
FLUORENE = 19.51
BAROMETRIC PRESSURE/ BARS =1.0202018
P CORRECTION/ BARS = 4.36794E-03
H20 VAPOR PRESS/ BARS = .03778776
WTM SEC/REV AVERAGE=76.8 WTM TEMP/K=300.372223
KGMS OF CATALYST =7.02570001E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.0101392 REACTOR TEMP/K=642.594444
INITIAL WTM M3 = 0 FINAL M3 = .0708
WTM TEMP/DEG K DURING M.B.=300.927778
KGS/SEC IN COND A=1.533456E-06 KGS/SEC IN B = 3.238E-07
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =663
GC AREA COUNTS, GAS 4 =4206 GAS 5 =7191
GC AREA COUNTS, GAS 6 =2194 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.045	27	4.791	1	.585	27	.169
2	.171	28	0	2	.613	28	0
3	.167	29	30.235	3	5.452	29	2.126
4	.214	30	3.593	4	7.136	30	1.134
5	.088	31	3.624	5	2.862	31	0
6	2.373	32	6.213	6	33.971	32	0
7	.936	33	1.574	7	8.481	33	0
8	0	34	3.534	8	3.187	34	0
9	1.107	35	.176	9	7.573	35	0
10	1.207	36	.465	10	4.728	36	0
11	.311	37	.818	11	1.106	37	0
12	.064	38	1.046	12	.21	38	0
13	.024	39	1.952	13	.077	39	0
14	3.442	40	.798	14	15.806	40	0
15	.252	41	.501	15	.424	41	0
16	.153	42	.408	16	.273	42	0
17	.118	43	.325	17	.132	43	0
18	.169	44	.606	18	.074	44	0
19	1.045	45	.139	19	.277	45	0
20	4.583	46	.429	20	2.181	46	0
21	1.998	47	.262	21	.408	47	0
22	2.678	48	1.95	22	0	48	0
23	4.892	49	.662	23	0	49	0
24	4.213	50	.73	24	.22	50	0
25	1.685	51	0	25	0	51	0
26	3.235	52	0	26	.174	52	0
		53	0			53	0

RUN NUMBER 74 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.51434362E-09	7.62358006E-07
C-DECALIN	8.6167735E-09	1.19126894E-06
TETRALIN	1.97771774E-10	2.61474062E-08
FLUORENE	2.88697626E-09	4.79902065E-07

TOTAL KG-MOLE FED/S = 1.72158652E-08
TOTAL KGS FED/S = 2.45967641E-06
PUMP RATE/ M3/S = 2.84262258E-09
TOTAL KG-ATOMS CARBON= 6.50945282E-04
TOTAL KG-ATOMS HYDROGEN= 1.02816305E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.9282407
WHSV (1/S) LIQ FEED BASIS= 3.50094187E-04
VHSV (1/S) = 2.18661526E-04
TOTAL WHSV (1/S) = 5.55575538E-04
MOLAR GAS DENSITY =.280890919 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.94097415
SUPERFICIAL GAS VELOCITY/ M/S = .0134237761

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.5333456E-06 KGS/S,COND B= 3.2375259E-07
KG-MOLE/S OF ALL GAS OUT= 7.22191784E-07
H2 FEEDRATE KG-MOLE/S = 7.21830938E-07
FRACTION OF GAS THAT IS HYDROCARBONS =7.04299696E-03
KG-MOLE/S FREE H2 IN GAS= 7.1710539E-07
H BALANCE CLOSURE = 97.7968588 C BALANCE CLOSURE=85.6246616

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	2.25307224E-03	1	.354550866
2	8.8343813E-04	2	.139020733
3	2.03086491E-04	3	.0319583589
4	1.58125621E-03	4	.248831684
5	0	5	0
6	4.81400015E-04	6	.0757546913
7	1.29530289E-03	7	0
8	1.61784041E-04	8	0
9	6.94810752E-05	9	0
10	5.34224693E-04	10	.0840673566
11	3.14559771E-04	11	.0495001613
12	8.00486078E-05	12	.0125967125
13	6.8462273E-05	13	0
14	2.36359844E-05	14	3.71943632E-03
H2	.272941166		

KG-MOLE FLUORENE/S IN PRODUCT = 1.79872702E-10
FLUORENE CONVERSION = 93.7695123 %
T-DECALIN CONVERSION= 38.2848978 %
C-DECALIN CONVERSION= 95.0470702 %

RUN NUMBER =75 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN75TP
PUMP TEMP/ DEG K =388.15
INITIAL TIME OF M. B./S =8707.8 FINAL TIME=12399
INITIAL PUMP VOL/M3= 1.8661E-04 FINAL VOL/M3= 1.971E-04
WT % OF TRANS-DECALIN =30.993
CIS-DECALIN = 48.43
TETRALIN = 1.063
FLUORENE = 19.51
BAROMETRIC PRESSURE/ BARS =1.0246036
P CORRECTION/ BARS = 4.38487E-03
H20 VAPOR PRESS/ BARS = .03474036
WTM SEC/REV AVERAGE=77.7 WTM TEMP/K=298.705556
KGMS OF CATALYST =7.483E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=672.594445
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.538889
KGS/SEC IN COND A=2.05674786E-06 KGS/SEC IN B =1.044E-07
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =406
GC AREA COUNTS, GAS 4 =2709 GAS 5 =4479
GC AREA COUNTS, GAS 6 =1035 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.018	27	2.094	1	.269	27	0
2	.071	28	2.935	2	.277	28	0
3	.054	29	35.318	3	2.523	29	2.665
4	.103	30	14.975	4	4.889	30	.484
5	.033	31	2.85	5	1.754	31	.257
6	1.302	32	4.404	6	41.142	32	0
7	.369	33	1.12	7	6.875	33	0
8	0	34	3.498	8	0	34	0
9	.546	35	.044	9	10.103	35	0
10	.55	36	.112	10	6.729	36	0
11	.138	37	.153	11	1.564	37	0
12	0	38	.253	12	0	38	0
13	0	39	.967	13	0	39	0
14	1.072	40	.36	14	14.412	40	0
15	.086	41	.498	15	0	41	0
16	.06	42	.372	16	0	42	0
17	.068	43	.15	17	.11	43	0
18	.108	44	.381	18	0	44	0
19	.267	45	.077	19	.75	45	0
20	.875	46	.595	20	2.643	46	0
21	.481	47	.341	21	.652	47	0
22	1.507	48	8.47	22	.458	48	0
23	2.81	49	1.854	23	.197	49	0
24	1.337	50	2.867	24	0	50	0
25	1.2	51	0	25	.384	51	0
26	2.259	52	0	26	.46	52	0
		53	0			53	0

RUN NUMBER 75 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.491989E-09	7.59267479E-07
C-DECALIN	8.58184195E-09	1.18643965E-06
TETRALIN	1.96970026E-10	2.60414071E-08
FLUORENE	2.87527274E-09	4.77956588E-07

TOTAL KG-MOLE FED/S = 1.71460737E-08
TOTAL KGS FED/S = 2.44970512E-06
PUMP RATE/ M3/S = 2.84191697E-09
TOTAL KG-ATOMS CARBON= 6.48306413E-04
TOTAL KG-ATOMS HYDROGEN= 1.02399498E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.1612781
WHSV (1/S) LIQ FEED BASIS= 3.27366768E-04
VHSV (1/S) = 2.18607249E-04
TOTAL WHSV (1/S) = 5.20576604E-04
MOLAR GAS DENSITY =.264667448 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.6493086
SUPERFICIAL GAS VELOCITY/ M/S = .0142658912

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.05659979E-06 KGS/S,COND B= 1.04389724E-07
KG-MOLE/S OF ALL GAS OUT= 7.28389975E-07
H2 FEEDRATE KG-MOLE/S = 7.22900382E-07
FRACTION OF GAS THAT IS HYDROCARBONS =4.27902756E-03
KG-MOLE/S FREE H2 IN GAS= 7.25273175E-07
H BALANCE CLOSURE = 99.3208967 C BALANCE CLOSURE=94.8263242

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	1.1809173E-03	1	.309655814
2	4.00367749E-04	2	.104982967
3	7.67573457E-05	3	.0201270304
4	8.27715448E-04	4	.217040517
5	0	5	0
6	3.24259781E-04	6	.0850262136
7	1.87431116E-03	7	0
8	7.92983411E-04	8	0
9	6.19161916E-05	9	0
10	4.29832811E-04	10	.112709187
11	2.96571503E-04	11	.0777658948
12	1.60970231E-04	12	.0422090252
13	3.72412735E-04	13	0
14	1.1625267E-04	14	.03048335
H2	.25775218		

KG-MOLE FLUORENE/S IN PRODUCT = 1.04790953E-09
FLUORENE CONVERSION = 63.5544302 %
T-DECALIN CONVERSION= 3.96903358 %
C-DECALIN CONVERSION= 73.9994307 %

RUN NUMBER =76 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN76TP
PUMP TEMP/ DEG K =385.927778
INITIAL TIME OF M. B./S =8538 FINAL TIME=12279
INITIAL PUMP VOL/M3= 2.2186E-04 FINAL VOL/M3= 2.3249E-04
WT % OF TRANS-DECALIN =30.993
CIS-DECALIN = 48.43
TETRALIN = 1.063
FLUORENE = 19.51
BAROMETRIC PRESSURE/ BARS =1.0269738
P CORRECTION/ BARS = 4.60496E-03
H20 VAPOR PRESS/ BARS = .035227944
WTM SEC/REV AVERAGE=77.7 WTM TEMP/K=299.816667
KGMS OF CATALYST =6.9998E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.1480392 REACTOR TEMP/K=639.538889
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.816667
KGS/SEC IN COND A=2.01510564E-06 KGS/SEC IN B = 1.426E-07
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =349
GC AREA COUNTS, GAS 4 =2373 GAS 5 =4137
GC AREA COUNTS, GAS 6 =1023 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.061	27	2.658	1	.364	27	1.55
2	.026	28	3.771	2	.482	28	0
3	.042	29	36.822	3	4.6	29	7.776
4	.065	30	12.792	4	4.08	30	2.437
5	.021	31	2.284	5	1.4	31	0
6	.951	32	3.503	6	33	32	0
7	.271	33	1.432	7	4.464	33	0
8	0	34	2.556	8	2.601	34	0
9	.425	35	.066	9	8.466	35	0
10	.478	36	.136	10	6.745	36	0
11	.115	37	.142	11	1.399	37	0
12	0	38	.311	12	.197	38	0
13	0	39	.829	13	0	39	0
14	.671	40	.325	14	9.664	40	0
15	.088	41	.548	15	.776	41	0
16	.049	42	.376	16	.435	42	0
17	.045	43	.12	17	.287	43	0
18	.105	44	.469	18	.21	44	0
19	.202	45	.097	19	.909	45	0
20	.508	46	.689	20	3.425	46	0
21	.456	47	.333	21	1.071	47	0
22	2.558	48	6.544	22	.549	48	0
23	4.499	49	1.932	23	0	49	0
24	1.516	50	2.554	24	1.032	50	0
25	1.809	51	0	25	0	51	0
26	3.753	52	0	26	.985	52	0
		53	0			53	0

RUN NUMBER 76 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.50321561E-09	7.60819558E-07
C-DECALIN	8.59938476E-09	1.18886494E-06
TETRALIN	1.97372668E-10	2.60946404E-08
FLUORENE	2.88115031E-09	4.78933616E-07

TOTAL KG-MOLE FED/S = 1.71811234E-08
TOTAL KGS FED/S = 2.45471276E-06
PUMP RATE/ M3/S = 2.84150895E-09
TOTAL KG-ATOMS CARBON= 6.49631667E-04
TOTAL KG-ATOMS HYDROGEN= 1.02608821E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.9901535
WHSV (1/S) LIQ FEED BASIS= 3.50680465E-04
VHSV (1/S) = 2.18575863E-04
TOTAL WHSV (1/S) = 5.56809851E-04
MOLAR GAS DENSITY =.284825418 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =5.01308442
SUPERFICIAL GAS VELOCITY/ M/S = .013230683

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.01496056E-06 KGS/S,COND B= 1.42584474E-07
KG-MOLE/S OF ALL GAS OUT= 7.19239559E-07
H2 FEEDRATE KG-MOLE/S = 7.21438007E-07
FRACTION OF GAS THAT IS HYDROCARBONS =3.89466868E-03
KG-MOLE/S FREE H2 IN GAS= 7.16438359E-07
H BALANCE CLOSURE = 98.5092227 C BALANCE CLOSURE=93.6467

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	1.18692358E-03	1	.282685095
2	4.17847662E-04	2	.0995171952
3	1.07440055E-04	3	.0255885911
4	1.05172352E-03	4	.250485007
5	0	5	0
6	5.12152948E-04	6	.121977528
7	2.10896637E-03	7	0
8	7.31601274E-04	8	0
9	8.45014644E-05	9	0
10	3.76437619E-04	10	.089654722
11	2.53537255E-04	11	.0603840079
12	1.82142765E-04	12	.0433802526
13	3.07127998E-04	13	0
14	1.10542973E-04	14	.0263276013
H2	.277394472		

KG-MOLE FLUORENE/S IN PRODUCT = 7.93232385E-10
FLUORENE CONVERSION = 72.4682055 %
T-DECALIN CONVERSION= 1.02302982 %
C-DECALIN CONVERSION= 78.0270636 %

RUN NUMBER =77 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN77TP
PUMP TEMP/ DEG K =377.594445
INITIAL TIME OF M. B./S =9818.4 FINAL TIME=13554.6
INITIAL PUMP VOL/M3= 5.394E-05 FINAL VOL/M3= 6.455E-05
WT % OF TRANS-DECALIN =31.239
CIS-DECALIN = 47.962
TETRALIN = 1.04
FLUORENE = 19.759
BAROMETRIC PRESSURE/ BARS =1.024265
P CORRECTION/ BARS = 4.30022E-03
H20 VAPOR PRESS/ BARS = .035227944
WTM SEC/REV AVERAGE=77.85 WTM TEMP/K=299.261111
KGMS OF CATALYST =7.0215E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.0101392 REACTOR TEMP/K=667.038889
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.816667
KGS/SEC IN COND A=1.8532038E-06 KGS/SEC IN B = 1.456E-07
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =662
GC AREA COUNTS, GAS 4 =5351 GAS 5 =7863
GC AREA COUNTS, GAS 6 =2380 GAS 7 =1522

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.14	27	3.57	1	.258	27	.768
2	.067	28	3.114	2	.258	28	0
3	.109	29	34.469	3	2.922	29	3.885
4	.171	30	5.898	4	5.826	30	1.603
5	.061	31	3.594	5	2.155	31	.185
6	1.986	32	5.72	6	35.414	32	.279
7	.604	33	1.224	7	8.778	33	.199
8	0	34	4.173	8	2.592	34	0
9	.866	35	.121	9	7.952	35	0
10	.912	36	.292	10	4.869	36	0
11	.227	37	.381	11	1.121	37	0
12	.03	38	.578	12	.141	38	0
13	0	39	1.732	13	0	39	0
14	2.042	40	.829	14	14.414	40	0
15	.127	41	.733	15	.279	41	0
16	.084	42	.536	16	.214	42	0
17	.072	43	.308	17	.103	43	0
18	.161	44	.656	18	.069	44	0
19	.525	45	.17	19	.489	45	0
20	1.651	46	.87	20	2.151	46	0
21	.947	47	.481	21	.441	47	0
22	1.74	48	4.006	22	.466	48	0
23	3.808	49	1.54	23	.712	49	0
24	2.245	50	2.118	24	.394	50	0
25	1.515	51	0	25	.571	51	0
26	2.801	52	0	26	.476	52	0
		53	0			53	0

RUN NUMBER 77 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.59113537E-09	7.72974465E-07
C-DECALIN	8.58420676E-09	1.18676658E-06
TETRALIN	1.94642224E-10	2.57336484E-08
FLUORENE	2.94119339E-09	4.88914577E-07

TOTAL KG-MOLE FED/S = 1.73111777E-08
TOTAL KGS FED/S = 2.47438927E-06
PUMP RATE/ M3/S = 2.83980645E-09
TOTAL KG-ATOMS CARBON= 6.54962048E-04
TOTAL KG-ATOMS HYDROGEN= 1.03284541E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.5700779
WHSV (1/S) LIQ FEED BASIS= 3.52398986E-04
VHSV (1/S) = 2.18444903E-04
TOTAL WHSV (1/S) = 5.57375487E-04
MOLAR GAS DENSITY =.270600161 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.77357573
SUPERFICIAL GAS VELOCITY/ M/S = .0138945173

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.85307038E-06 KGS/S,COND B= 1.45612276E-07
KG-MOLE/S OF ALL GAS OUT= 7.18409717E-07
H2 FEEDRATE KG-MOLE/S = 7.19627008E-07
FRACTION OF GAS THAT IS HYDROCARBONS =8.62945634E-03
KG-MOLE/S FREE H2 IN GAS= 7.12210231E-07
H BALANCE CLOSURE = 98.6617028 C BALANCE CLOSURE=93.6187881

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	2.41430485E-03	1	.413272927
	2	5.31414935E-04	2	.0909658967
	3	1.20523374E-04	3	.0206308029
	4	1.13348191E-03	4	.194025781
	5	0	5	0
	6	4.47321115E-04	6	.0765709874
	7	1.71802355E-03	7	0
	8	2.97613893E-04	8	0
	9	6.40422253E-05	9	0
	10	5.47157536E-04	10	.0936606643
	11	3.95856494E-04	11	.0677614394
	12	1.71595964E-04	12	.0293732444
	13	1.64602966E-04	13	0
	14	8.02577164E-05	14	.0137382573
	H2	.262513964		

KG-MOLE FLUORENE/S IN PRODUCT = 4.4657402E-10
FLUORENE CONVERSION = 84.8165706 %
T-DECALIN CONVERSION= 16.6347798 %
C-DECALIN CONVERSION= 90.5939166 %

RUN NUMBER =78 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN78TP
PUMP TEMP/ DEG K =387.594445
INITIAL TIME OF M. B./S =12384.6 FINAL TIME=16243.8
INITIAL PUMP VOL/M3= 1.0234E-04 FINAL VOL/M3= 1.1331E-04
WT % OF TRANS-DECALIN =31.239
CIS-DECALIN = 47.962
TETRALIN = 1.04
FLUORENE = 19.759
BAROMETRIC PRESSURE/ BARS =1.0239264
P CORRECTION/ BARS = 4.96049E-03
H20 VAPOR PRESS/ BARS = .036490922
WTM SEC/REV AVERAGE=77.4 WTM TEMP/K=299.261111
KGMS OF CATALYST =7.0033E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.0790892 REACTOR TEMP/K=649.8
INITIAL WTM M3 = 0 FINAL M3 = .0708
WTM TEMP/DEG K DURING M.B.=300.65
KGS/SEC IN COND A=2.10222372E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =541
GC AREA COUNTS, GAS 4 =3450 GAS 5 =4936
GC AREA COUNTS, GAS 6 =1507 GAS 7 =575

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.107	27	3.427	1	0	27	0
2	.072	28	3.928	2	0	28	0
3	.313	29	33.838	3	0	29	0
4	.424	30	6.305	4	0	30	0
5	.155	31	2.536	5	0	31	0
6	3.452	32	4.042	6	0	32	0
7	.754	33	1.267	7	0	33	0
8	.304	34	2.734	8	0	34	0
9	1.248	35	.074	9	0	35	0
10	1.138	36	.166	10	0	36	0
11	.263	37	.175	11	0	37	0
12	.042	38	.351	12	0	38	0
13	.011	39	1.002	13	0	39	0
14	2.408	40	.364	14	0	40	0
15	.163	41	.933	15	0	41	0
16	.099	42	.157	16	0	42	0
17	.08	43	.05	17	0	43	0
18	.155	44	.375	18	0	44	0
19	.399	45	.085	19	0	45	0
20	1.393	46	.878	20	0	46	0
21	.767	47	.503	21	0	47	0
22	1.918	48	5.024	22	0	48	0
23	4.76	49	1.784	23	0	49	0
24	1.974	50	2.147	24	0	50	0
25	1.864	51	0	25	0	51	0
26	3.594	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 78 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.54262145E-09	7.66267416E-07
C-DECALIN	8.50972215E-09	1.17646909E-06
TETRALIN	1.92953326E-10	2.55103593E-08
FLUORENE	2.91567284E-09	4.84672297E-07

TOTAL KG-MOLE FED/S = 1.71609698E-08
TOTAL KGS FED/S = 2.45291916E-06
PUMP RATE/ M3/S = 2.84258078E-09
TOTAL KG-ATOMS CARBON= 6.49278984E-04
TOTAL KG-ATOMS HYDROGEN= 1.02388348E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.0808597
WHSV (1/S) LIQ FEED BASIS= 3.50249102E-04
VHSV (1/S) = 2.18658311E-04
TOTAL WHSV (1/S) = 5.56478332E-04
MOLAR GAS DENSITY =.279045838 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.90677551
SUPERFICIAL GAS VELOCITY/ M/S = .0135173355

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.10207237E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.20825949E-07
H2 FEEDRATE KG-MOLE/S = 7.2214836E-07
FRACTION OF GAS THAT IS HYDROCARBONS =5.41626857E-03
KG-MOLE/S FREE H2 IN GAS= 7.16921762E-07
H BALANCE CLOSURE = 98.601749 C BALANCE CLOSURE=93.7979472

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	1.5904605E-03	1	.316821039
	2	4.70624296E-04	2	.0937487466
	3	1.3820262E-04	3	.0275300756
	4	1.23225557E-03	4	.245466323
	5	0	5	0
	6	5.78531903E-04	6	.115244031
	7	1.94770297E-03	7	0
	8	3.62913506E-04	8	0
	9	7.62597698E-05	9	0
	10	4.3761512E-04	10	.0871732916
	11	2.7231141E-04	11	.0542446567
	12	2.05273109E-04	12	.040890572
	13	2.4050461E-04	13	0
	14	9.47850735E-05	14	.0188812645
	H2	.271398398		

KG-MOLE FLUORENE/S IN PRODUCT = 6.35313216E-10
FLUORENE CONVERSION = 78.2104081 %
T-DECALIN CONVERSION= 7.17349661 %
C-DECALIN CONVERSION= 88.7344543 %

RUN NUMBER =79 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN79TP
PUMP TEMP/ DEG K =390.372222
INITIAL TIME OF M. B./S =8092.8 FINAL TIME=11860.8
INITIAL PUMP VOL/M3= 1.3969E-04 FINAL VOL/M3= 1.504E-04
WT % OF TRANS-DECALIN =31.24
CIS-DECALIN = 47.96
TETRALIN = 1.04
FLUORENE = 19.76
BAROMETRIC PRESSURE/ BARS =1.0188474
P CORRECTION/ BARS = 5.18058E-03
H20 VAPOR PRESS/ BARS = .03650108
WTM SEC/REV AVERAGE=69.6 WTM TEMP/K=300.372223
KGMS OF CATALYST =7.0011E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.1480392 REACTOR TEMP/K=655.372223
INITIAL WTM M3 = 0 FINAL M3 = .073632
WTM TEMP/DEG K DURING M.B.=300.372223
KGS/SEC IN COND A=2.05624782E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =602
GC AREA COUNTS, GAS 4 =3590 GAS 5 =5900
GC AREA COUNTS, GAS 6 =1511 GAS 7 =923

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.192	27	3.099	1	0	27	0
2	.112	28	3.269	2	0	28	0
3	.425	29	31.775	3	0	29	0
4	.624	30	5.21	4	0	30	0
5	.214	31	2.679	5	0	31	0
6	5.538	32	4.234	6	0	32	0
7	.965	33	1.086	7	0	33	0
8	.373	34	3.05	8	0	34	0
9	1.724	35	.061	9	0	35	0
10	1.485	36	.157	10	0	36	0
11	.347	37	.188	11	0	37	0
12	.054	38	.332	12	0	38	0
13	.013	39	1.059	13	0	39	0
14	2.594	40	.386	14	0	40	0
15	.185	41	.699	15	0	41	0
16	.114	42	.652	16	0	42	0
17	.092	43	.422	17	0	43	0
18	.155	44	.842	18	0	44	0
19	.421	45	.037	19	0	45	0
20	1.288	46	.526	20	0	46	0
21	.747	47	.292	21	0	47	0
22	1.88	48	5.183	22	0	48	0
23	4.361	49	1.687	23	0	49	0
24	1.835	50	2.536	24	0	50	0
25	1.665	51	0	25	0	51	0
26	3.139	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 79 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.52718552E-09	7.64133398E-07
C-DECALIN	8.48539749E-09	1.1731062E-06
TETRALIN	1.92409801E-10	2.54384998E-08
FLUORENE	2.90760691E-09	4.83331496E-07

TOTAL KG-MOLE FED/S = 1.71125997E-08
TOTAL KGS FED/S = 2.4460096E-06
PUMP RATE/ M3/S = 2.84237942E-09
TOTAL KG-ATOMS CARBON= 6.47450565E-04
TOTAL KG-ATOMS HYDROGEN= 1.02099316E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 46.5029375
WHSV (1/S) LIQ FEED BASIS= 3.49372246E-04
VHSV (1/S) = 2.18642822E-04
TOTAL WHSV (1/S) = 5.76702177E-04
MOLAR GAS DENSITY =.27794616 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.44499264
SUPERFICIAL GAS VELOCITY/ M/S = .0149216289

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.05609978E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.64360205E-07
H2 FEEDRATE KG-MOLE/S = 7.95786156E-07
FRACTION OF GAS THAT IS HYDROCARBONS =6.1077114E-03
KG-MOLE/S FREE H2 IN GAS= 7.59691714E-07
H BALANCE CLOSURE = 95.5786618 C BALANCE CLOSURE=93.8305914
PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	1.81485663E-03	1	.348738912
2	6.58072029E-04	2	.126453693
3	1.61237218E-04	3	.0309829939
4	1.08247466E-03	4	.208005981
5	0	5	0
6	4.83207957E-04	6	.0928521925
7	1.68262278E-03	7	0
8	2.75891886E-04	8	0
9	6.01356299E-05	9	0
10	4.19749715E-04	10	.0806581945
11	3.10896069E-04	11	.0597411141
12	1.70560425E-04	12	.0327745211
13	2.28264381E-04	13	0
14	1.03000734E-04	14	.0197923976
H2	.27049519		

KG-MOLE FLUORENE/S IN PRODUCT = 6.41085554E-10
FLUORENE CONVERSION = 77.9514365 %
T-DECALIN CONVERSION= 14.5010927 %
C-DECALIN CONVERSION= 90.8684484 %

RUN NUMBER =80 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN80PR
PUMP TEMP/ DEG K =389.816667
INITIAL TIME OF M. B./S =8615.4 FINAL TIME=12331.2
INITIAL PUMP VOL/M3= 1.7086E-04 FINAL VOL/M3= 1.8142E-04
WT % OF TRANS-DECALIN =31.24
CIS-DECALIN = 47.96
TETRALIN = 1.04
FLUORENE = 19.76
BAROMETRIC PRESSURE/ BARS =1.019186
P CORRECTION/ BARS = 4.84198E-03
H20 VAPOR PRESS/ BARS = .039589112
WTM SEC/REV AVERAGE=77.7 WTM TEMP/K=300.65
KGMS OF CATALYST =7.001E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=35.9019892 REACTOR TEMP/K=661.15
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=301.761111
KGS/SEC IN COND A=2.22923388E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =574
GC AREA COUNTS, GAS 4 =4052 GAS 5 =7315
GC AREA COUNTS, GAS 6 =2100 GAS 7 =1793

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.343	27	3.893	1	0	27	0
2	.183	28	4.003	2	0	28	0
3	.474	29	27.937	3	0	29	0
4	.769	30	3.144	4	0	30	0
5	.289	31	2.376	5	0	31	0
6	4.721	32	3.52	6	0	32	0
7	.692	33	2.005	7	0	33	0
8	.364	34	2.334	8	0	34	0
9	1.506	35	.401	9	0	35	0
10	1.333	36	.585	10	0	36	0
11	.322	37	.555	11	0	37	0
12	.068	38	.898	12	0	38	0
13	.023	39	1.392	13	0	39	0
14	1.238	40	.816	14	0	40	0
15	.248	41	1.219	15	0	41	0
16	.162	42	1.146	16	0	42	0
17	.175	43	.557	17	0	43	0
18	.324	44	.094	18	0	44	0
19	.473	45	0	19	0	45	0
20	.874	46	.727	20	0	46	0
21	1.03	47	.326	21	0	47	0
22	3.932	48	3.792	22	0	48	0
23	8.722	49	1.714	23	0	49	0
24	0	50	1.411	24	0	50	0
25	2.381	51	0	25	0	51	0
26	4.513	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 80 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.52938769E-09	7.64437849E-07
C-DECALIN	8.48877829E-09	1.1735736E-06
TETRALIN	1.92486462E-10	2.54486352E-08
FLUORENE	2.90876538E-09	4.83524068E-07

TOTAL KG-MOLE FED/S = 1.71194178E-08
TOTAL KGS FED/S = 2.44698415E-06
PUMP RATE/ M3/S = 2.84194101E-09
TOTAL KG-ATOMS CARBON= 6.47708526E-04
TOTAL KG-ATOMS HYDROGEN= 1.02139995E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.4974692
WHSV (1/S) LIQ FEED BASIS= 3.49516437E-04
VHSV (1/S) = 2.18609099E-04
TOTAL WHSV (1/S) = 5.52460826E-04
MOLAR GAS DENSITY =.652991139 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =11.6681514
SUPERFICIAL GAS VELOCITY/ M/S = 5.68440779E-03

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.22907339E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.10426973E-07
H2 FEEDRATE KG-MOLE/S = 7.10412514E-07
FRACTION OF GAS THAT IS HYDROCARBONS =7.58318357E-03
KG-MOLE/S FREE H2 IN GAS= 7.05039675E-07
H BALANCE CLOSURE = 100.430071 C BALANCE CLOSURE=102.533333

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	5.39012127E-03	1	.351820741
	2	1.59665598E-03	2	.104215965
	3	4.33287869E-04	3	.0282813042
	4	2.96422101E-03	4	.193478844
	5	0	5	0
	6	2.16882225E-03	6	.141562056
	7	4.04043659E-03	7	0
	8	4.54706398E-04	8	0
	9	3.03224116E-04	9	0
	10	1.22521586E-03	10	.0799715501
	11	7.62706069E-04	11	.04978289
	12	6.23097987E-04	12	.0406704755
	13	4.56113148E-04	13	0
	14	1.56518403E-04	14	.0102161747
	H2	.632416012		

KG-MOLE FLUORENE/S IN PRODUCT = 5.08491024E-10
FLUORENE CONVERSION = 82.5186649 %
T-DECALIN CONVERSION= 18.5367086 %
C-DECALIN CONVERSION= 94.0283194 %

RUN NUMBER =81 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN81PR
PUMP TEMP/ DEG K =390.372222
INITIAL TIME OF M. B./S =7348.2 FINAL TIME=11025.6
INITIAL PUMP VOL/M3= 2.033E-04 FINAL VOL/M3= 2.1374E-04
WT % OF TRANS-DECALIN =31.24
CIS-DECALIN = 47.96
TETRALIN = 1.04
FLUORENE = 19.76
BAROMETRIC PRESSURE/ BARS =1.0168158
P CORRECTION/ BARS = 4.2325E-03
H20 VAPOR PRESS/ BARS = .033071062
WTM SEC/REV AVERAGE=77.4 WTM TEMP/K=298.427778
KGMS OF CATALYST =7.0004E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=7.90828921 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=298.705556
KGS/SEC IN COND A=2.04746934E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =195
GC AREA COUNTS, GAS 4 =3085 GAS 5 =6362
GC AREA COUNTS, GAS 6 =1082 GAS 7 =1363

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.051	27	1.836	1	0	27	0
2	.028	28	3.108	2	0	28	0
3	.127	29	33.732	3	0	29	0
4	.245	30	10.607	4	0	30	0
5	.083	31	3.047	5	0	31	0
6	2.367	32	5.706	6	0	32	0
7	.294	33	0	7	0	33	0
8	0	34	3.772	8	0	34	0
9	.661	35	.42	9	0	35	0
10	.54	36	.301	10	0	36	0
11	.107	37	.407	11	0	37	0
12	.016	38	0	12	0	38	0
13	0	39	1.098	13	0	39	0
14	.884	40	.529	14	0	40	0
15	.074	41	.848	15	0	41	0
16	.045	42	.615	16	0	42	0
17	.055	43	.264	17	0	43	0
18	.101	44	.522	18	0	44	0
19	.174	45	.026	19	0	45	0
20	.529	46	.317	20	0	46	0
21	.382	47	.183	21	0	47	0
22	1.795	48	10.315	22	0	48	0
23	4.614	49	2.04	23	0	49	0
24	0	50	2.845	24	0	50	0
25	1.514	51	0	25	0	51	0
26	2.776	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 81 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.52058486E-09	7.63220857E-07
C-DECALIN	8.47526409E-09	1.17170526E-06
TETRALIN	1.92180022E-10	2.54081207E-08
FLUORENE	2.90413459E-09	4.82754294E-07

TOTAL KG-MOLE FED/S = 1.70921636E-08
TOTAL KGS FED/S = 2.44308853E-06
PUMP RATE/ M3/S = 2.838985E-09
TOTAL KG-ATOMS CARBON= 6.46677369E-04
TOTAL KG-ATOMS HYDROGEN= 1.01977388E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.2404026
WHSV (1/S) LIQ FEED BASIS= 3.48989913E-04
VHSV (1/S) = 2.18381715E-04
TOTAL WHSV (1/S) = 5.55256439E-04
MOLAR GAS DENSITY =.143589494 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =2.5309825
SUPERFICIAL GAS VELOCITY/ M/S = .0262058433

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.04732193E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.26723221E-07
H2 FEEDRATE KG-MOLE/S = 7.21979871E-07
FRACTION OF GAS THAT IS HYDROCARBONS =5.73276375E-03
KG-MOLE/S FREE H2 IN GAS= 7.24545623E-07
H BALANCE CLOSURE = 99.0397464 C BALANCE CLOSURE=93.2597637

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	8.35533971E-04	1	.376594072
2	1.48076525E-04	2	.0667414415
3	2.63323561E-05	3	.0118685889
4	3.4639404E-04	4	.156127634
5	0	5	0
6	2.281366E-04	6	.102826329
7	9.66286259E-04	7	0
8	3.0384793E-04	8	0
9	0	9	0
10	2.92746725E-04	10	.131947575
11	1.82885899E-04	11	.0824308138
12	9.60452338E-05	12	.0432897607
13	2.45747258E-04	13	0
14	6.25080355E-05	14	.0281737864
H2	.140154953		

KG-MOLE FLUORENE/S IN PRODUCT = 1.27041603E-09
FLUORENE CONVERSION = 56.2549189 %
T-DECALIN CONVERSION= 9.51470627 %
C-DECALIN CONVERSION= 81.4663768 %

RUN NUMBER =82 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN82TP
PUMP TEMP/ DEG K =383.705556
INITIAL TIME OF M. B./S =8536.2 FINAL TIME=12243.6
INITIAL PUMP VOL/M3= 6.545E-05 FINAL VOL/M3= 7.598E-05
WT % OF TRANS-DECALIN =30.283
CIS-DECALIN = 46.31
TETRALIN = 1.01
FLUORENE = 22.397
BAROMETRIC PRESSURE/ BARS =1.0202018
P CORRECTION/ BARS = 4.36794E-03
H20 VAPOR PRESS/ BARS = .03890514
WTM SEC/REV AVERAGE=78 WTM TEMP/K=300.094445
KGMS OF CATALYST =7.0023E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.1480392 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=301.483334
KGS/SEC IN COND A=2.2717095E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =806
GC AREA COUNTS, GAS 4 =4806 GAS 5 =8272
GC AREA COUNTS, GAS 6 =1991 GAS 7 =1577

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.13	27	2.46	1	0	27	0
2	.069	28	3.456	2	0	28	0
3	.203	29	33.164	3	0	29	0
4	.344	30	7.896	4	0	30	0
5	.11	31	2.556	5	0	31	0
6	3.188	32	3.98	6	0	32	0
7	.534	33	.996	7	0	33	0
8	0	34	2.892	8	0	34	0
9	1	35	.048	9	0	35	0
10	.828	36	.139	10	0	36	0
11	.182	37	.196	11	0	37	0
12	.017	38	.379	12	0	38	0
13	0	39	1.156	13	0	39	0
14	1.306	40	.577	14	0	40	0
15	.107	41	1.493	15	0	41	0
16	.071	42	1.075	16	0	42	0
17	.083	43	1.181	17	0	43	0
18	.13	44	.069	18	0	44	0
19	.254	45	0	19	0	45	0
20	.716	46	.721	20	0	46	0
21	.488	47	.444	21	0	47	0
22	1.586	48	8.754	22	0	48	0
23	3.958	49	2.159	23	0	49	0
24	1.416	50	2.681	24	0	50	0
25	1.616	51	0	25	0	51	0
26	3.191	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 82 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.42569545E-09	7.50102395E-07
C-DECALIN	8.29719499E-09	1.14708721E-06
TETRALIN	1.89225092E-10	2.50174494E-08
FLUORENE	3.33735266E-09	5.54768132E-07

TOTAL KG-MOLE FED/S = 1.72494682E-08
TOTAL KGS FED/S = 2.47697518E-06
PUMP RATE/ M3/S = 2.84028813E-09
TOTAL KG-ATOMS CARBON= 6.57019008E-04
TOTAL KG-ATOMS HYDROGEN= 1.01755438E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.193768
WHSV (1/S) LIQ FEED BASIS= 3.5373454E-04
VHSV (1/S) = 2.18481955E-04
TOTAL WHSV (1/S) = 5.566864E-04
MOLAR GAS DENSITY =.275610478 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.92287185
SUPERFICIAL GAS VELOCITY/ M/S = .0134731378

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.27154595E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.14281647E-07
H2 FEEDRATE KG-MOLE/S = 7.1057059E-07
FRACTION OF GAS THAT IS HYDROCARBONS =8.46077978E-03
KG-MOLE/S FREE H2 IN GAS= 7.08238268E-07
H BALANCE CLOSURE = 100.9u5897 C BALANCE CLOSURE=104.376687
PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	2.3758681E-03	1	.419713785
2	4.43932143E-04	2	.0784237307
3	8.66771224E-05	3	.0153121224
4	9.84598735E-04	4	.173936281
5	0	5	0
6	4.97444555E-04	6	.0878770741
7	2.05342933E-03	7	0
8	4.88899951E-04	8	0
9	6.44871268E-05	9	0
10	4.67793013E-04	10	.0826389211
11	3.70354551E-04	11	.0654257323
12	3.0669729E-04	12	.0541802301
13	4.50790891E-04	13	0
14	1.27320852E-04	14	.0224921226
H2	.266892184		

KG-MOLE FLUORENE/S IN PRODUCT = 1.19624095E-09
FLUORENE CONVERSION = 64.1559922 %
T-DECALIN CONVERSION= -.431021748 %
C-DECALIN CONVERSION= 84.3637636 %

RUN NUMBER =83 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN83PR
PUMP TEMP/ DEG K =387.594445
INITIAL TIME OF M. B./S =8647.8 FINAL TIME=12342.6
INITIAL PUMP VOL/M3= 1.0768E-04 FINAL VOL/M3= 1.1818E-04
WT % OF TRANS-DECALIN =30.283
CIS-DECALIN = 46.31
TETRALIN = 1.01
FLUORENE = 22.397
BAROMETRIC PRESSURE/ BARS =1.0195246
P CORRECTION/ BARS = 4.7404E-03
H20 VAPOR PRESS/ BARS = .040049608
WTM SEC/REV AVERAGE=78 WTM TEMP/K=301.761111
KGMS OF CATALYST =6.9999E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=25.1457892 REACTOR TEMP/K=661.705556
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=302.038889
KGS/SEC IN COND A=1.68088446E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =1675
GC AREA COUNTS, GAS 4 =8190 GAS 5 =11421
GC AREA COUNTS, GAS 6 =3556 GAS 7 =2132

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.479	27	4.077	1	0	27	0
2	.326	28	4.775	2	0	28	0
3	1.248	29	21.454	3	0	29	0
4	1.429	30	2.573	4	0	30	0
5	.539	31	2.775	5	0	31	0
6	8.196	32	4.507	6	0	32	0
7	1.682	33	1.368	7	0	33	0
8	.788	34	3.048	8	0	34	0
9	2.498	35	.114	9	0	35	0
10	1.939	36	.256	10	0	36	0
11	.509	37	.345	11	0	37	0
12	.077	38	.578	12	0	38	0
13	.027	39	1.375	13	0	39	0
14	3.638	40	.512	14	0	40	0
15	.26	41	.942	15	0	41	0
16	.178	42	.831	16	0	42	0
17	.119	43	.615	17	0	43	0
18	.01	44	.993	18	0	44	0
19	.649	45	.046	19	0	45	0
20	2.237	46	.627	20	0	46	0
21	1.173	47	.369	21	0	47	0
22	2.433	48	2.679	22	0	48	0
23	4.659	49	1.314	23	0	49	0
24	2.591	50	1.527	24	0	50	0
25	1.696	51	0	25	0	51	0
26	2.924	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 83 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.4078722E-09	7.47638332E-07
C-DECALIN	8.26993896E-09	1.14331906E-06
TETRALIN	1.88603493E-10	2.49352678E-08
FLUORENE	3.32638955E-09	5.52945736E-07

TOTAL KG-MOLE FED/S = 1.71928042E-08
TOTAL KGS FED/S = 2.4688384E-06
PUMP RATE/ M3/S = 2.84185449E-09
TOTAL KG-ATOMS CARBON= 6.5486072E-04
TOTAL KG-ATOMS HYDROGEN= 1.01421174E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.0090929
WHSV (1/S) LIQ FEED BASIS= 3.52693417E-04
VHSV (1/S) = 2.18602443E-04
TOTAL WHSV (1/S) = 5.5414077E-04
MOLAR GAS DENSITY =.456973269 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =8.22522149
SUPERFICIAL GAS VELOCITY/ M/S = 8.06379873E-03

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.68076345E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.13793245E-07
H2 FEEDRATE KG-MOLE/S = 7.05061304E-07
FRACTION OF GAS THAT IS HYDROCARBONS =.0132676905
KG-MOLE/S FREE H2 IN GAS= 7.04322857E-07
H BALANCE CLOSURE = 99.5228398 C BALANCE CLOSURE=86.7280649

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	6.51452846E-03	1	.511900058
2	1.37807508E-03	2	.108286689
3	3.42775503E-04	3	.0269346892
4	2.16397213E-03	4	.170041081
5	0	5	0
6	7.9614352E-04	6	.0625595416
7	1.63731433E-03	7	0
8	1.9636477E-04	8	0
9	1.09171862E-04	9	0
10	6.74438849E-04	10	.052996205
11	5.05423334E-04	11	.0397152665
12	2.61433129E-04	12	.0205429503
13	1.70040446E-04	13	0
14	8.93825396E-05	14	7.02352096E-03
H2	.442134205		

KG-MOLE FLUORENE/S IN PRODUCT = 2.7087561E-10
FLUORENE CONVERSION = 91.8567683 %
T-DECALIN CONVERSION= 51.7693283 %
C-DECALIN CONVERSION= 96.2175 %

RUN NUMBER =84 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN84FR
PUMP TEMP/ DEG K =386.483333
INITIAL TIME OF M. B./S =11542.2 FINAL TIME=18886.2
INITIAL PUMP VOL/M3= 1.37E-04 FINAL VOL/M3= 1.4744E-04
WT % OF TRANS-DECALIN =30.283
CIS-DECALIN = 46.31
TETRALIN = 1.01
FLUORENE = 22.397
BAROMETRIC PRESSURE/ BARS =1.0256194
P CORRECTION/ BARS = 4.30022E-03
H20 VAPOR PRESS/ BARS = .02983066
WTM SEC/REV AVERAGE=77.4 WTM TEMP/K=298.427778
KGMS OF CATALYST =7.0407E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.0101392 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .135936
WTM TEMP/DEG K DURING M.B.=297.038889
KGS/SEC IN COND A=9.67355159E-07 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =452
GC AREA COUNTS, GAS 4 =2529 GAS 5 =4437
GC AREA COUNTS, GAS 6 =1068 GAS 7 =1089

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.109	27	3.336	1	0	27	0
2	.084	28	4.247	2	0	28	0
3	.402	29	24.548	3	0	29	0
4	.653	30	3.226	4	0	30	0
5	.21	31	3.705	5	0	31	0
6	6.169	32	5.757	6	0	32	0
7	.979	33	1.391	7	0	33	0
8	.421	34	4.452	8	0	34	0
9	1.697	35	.317	9	0	35	0
10	1.478	36	.526	10	0	36	0
11	.347	37	.65	11	0	37	0
12	.05	38	.92	12	0	38	0
13	0	39	2.279	13	0	39	0
14	2.72	40	1.253	14	0	40	0
15	.169	41	1.69	15	0	41	0
16	.11	42	1.085	16	0	42	0
17	.103	43	.652	17	0	43	0
18	.162	44	1.151	18	0	44	0
19	.478	45	.083	19	0	45	0
20	1.45	46	.521	20	0	46	0
21	.892	47	.348	21	0	47	0
22	1.613	48	4.49	22	0	48	0
23	3.433	49	1.894	23	0	49	0
24	1.958	50	2.019	24	0	50	0
25	1.331	51	0	25	0	51	0
26	2.445	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 84 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	2.70816369E-09	3.7440363E-07
C-DECALIN	4.14143449E-09	5.72553317E-07
TETRALIN	9.44491868E-11	1.2487127E-08
FLUORENE	1.66579517E-09	2.76905132E-07

TOTAL KG-MOLE FED/S = 8.60984253E-09
TOTAL KGS FED/S = 1.23634921E-06
PUMP RATE/ M3/S = 1.42158E-09
TOTAL KG-ATOMS CARBON= 3.27942296E-04
TOTAL KG-ATOMS HYDROGEN= 5.0789873E-04

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 84.8804561
WHSV (1/S) LIQ FEED BASIS= 1.7559892E-04
VHSV (1/S) = 1.09351433E-04
TOTAL WHSV (1/S) = 3.83192345E-04
MOLAR GAS DENSITY =.273101507 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.80154908
SUPERFICIAL GAS VELOCITY/ M/S = .0138135692

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 9.67285515E-07 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.42860259E-07
H2 FEEDRATE KG-MOLE/S = 7.30807361E-07
FRACTION OF GAS THAT IS HYDROCARBONS =4.61618213E-03
KG-MOLE/S FREE H2 IN GAS= 7.39431081E-07
H BALANCE CLOSURE = 100.73417 C BALANCE CLOSURE=92.6552705

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	1.31432122E-03	1	.410125234
2	3.41362523E-04	2	.106519915
3	7.91174456E-05	3	.0246880749
4	5.42029863E-04	4	.169136829
5	0	5	0
6	2.06215915E-04	6	.0643483105
7	6.24961515E-04	7	0
8	8.21299433E-05	8	0
9	3.70309731E-05	9	0
10	3.09983288E-04	10	.0967282322
11	2.53153507E-04	11	.0789948755
12	1.19074648E-04	12	.0371564555
13	9.50690679E-05	13	0
14	3.94242414E-05	14	.0123020734
H2	.269057633		

KG-MOLE FLUORENE/S IN PRODUCT = 2.61271248E-10
FLUORENE CONVERSION = 84.3155238 %
T-DECALIN CONVERSION= 36.5793413 %
C-DECALIN CONVERSION= 94.5499171 %

RUN NUMBER =85 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN85FR
PUMP TEMP/ DEG K =391.483333
INITIAL TIME OF M. B./S =14694 FINAL TIME=29397.6
INITIAL PUMP VOL/M3= 1.5783E-04 FINAL VOL/M3= 1.68E-04
WT % OF TRANS-DECALIN =30.283
CIS-DECALIN = 46.31
TETRALIN = 1.01
FLUORENE = 22.397
BAROMETRIC PRESSURE/ BARS =1.0269738
P CORRECTION/ BARS = 4.60496E-03
H20 VAPOR PRESS/ BARS = .03585774
WTM SEC/REV AVERAGE=77.7 WTM TEMP/K=298.427778
KGMS OF CATALYST =6.9979E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.1480392 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .271872
WTM TEMP/DEG K DURING M.B.=300.094445
KGS/SEC IN COND A=4.2686748E-07 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =285
GC AREA COUNTS, GAS 4 =1857 GAS 5 =3583
GC AREA COUNTS, GAS 6 =834 GAS 7 =629

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.045	27	3.819	1	0	27	0
2	.03	28	4.127	2	0	28	0
3	.227	29	21.117	3	0	29	0
4	.748	30	2.322	4	0	30	0
5	.25	31	4.626	5	0	31	0
6	8.001	32	7.349	6	0	32	0
7	1.759	33	1.457	7	0	33	0
8	0	34	4.653	8	0	34	0
9	2.144	35	.078	9	0	35	0
10	1.806	36	.26	10	0	36	0
11	.391	37	.417	11	0	37	0
12	.058	38	.573	12	0	38	0
13	.015	39	1.628	13	0	39	0
14	3.04	40	.616	14	0	40	0
15	.205	41	.51	15	0	41	0
16	.12	42	.397	16	0	42	0
17	.1	43	.234	17	0	43	0
18	.14	44	.594	18	0	44	0
19	.633	45	.078	19	0	45	0
20	1.724	46	.587	20	0	46	0
21	.857	47	.363	21	0	47	0
22	1.545	48	4.258	22	0	48	0
23	3.163	49	2.216	23	0	49	0
24	1.96	50	1.894	24	0	50	0
25	1.147	51	0	25	0	51	0
26	2.113	52	0	26	0	52	0
		53	3.606			53	0

```
RUN NUMBER  85   MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES
COMPOUND          KG-MOLE/SECOND          KG/S
T-DECALIN      1.31109386E-09          1.81258726E-07
C-DECALIN      2.00497825E-09          2.77188244E-07
TETRALIN      4.57253559E-11          6.0453493E-09
FLUORENE      8.06455616E-10          1.34057117E-07
TOTAL KG-MOLE FED/S =  4.16825308E-09
TOTAL   KGS FED/S =  5.98549436E-07
PUMP RATE/ M3/S  =  6.91672876E-10
TOTAL KG-ATOMS CARBON=   1.58765562E-04
TOTAL KG-ATOMS HYDROGEN=   2.45887243E-04


FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 173.773305
WHSV (1/S) LIQ FEED BASIS=  8.55320378E-05
VHSV (1/S) =       5.32051803E-05
TOTAL WHSV (1/S) = 2.92544233E-04
MOLAR GAS DENSITY =.275610478  KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC    =4.91828138
SUPERFICIAL GAS VELOCITY/  M/S   =    .0134857129


MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 4.26836748E-07  KGS/S,COND B= 0
KG-MOLE/S  OF ALL GAS OUT= 7.30833556E-07
H2 FEEDRATE KG-MOLE/S  = 7.24331114E-07
FRACTION OF GAS THAT IS HYDROCARBONS =3.46494083E-03
KG-MOLE/S FREE H2 IN GAS=  7.2830126E-07
H BALANCE CLOSURE = 100.591359  C BALANCE CLOSURE=92.9282818
                    PRODUCT DISTRIBUTION
          WITH FEEDSTOCK                WITHOUT FEEDSTOCK
COMPOUND GROUP CONC./KG-MOLE/M3   COMP. GROUP   MOLE FRAC.
        1       9.76122434E-04        1       .50779905
        2       1.98422537E-04        2       .103223502
        3       3.38210286E-05        3       .0175943976
        4       2.67319537E-04        4       .139065144
        5       4.37657297E-05        5       .0227678364
        6       9.42007511E-05        6       .0490051762
        7       2.44708729E-04        7       0
        8       2.69078785E-05        8       0
        9       1.76554027E-05        9       0
        10      1.59660102E-04        10      .0830584827
        11      9.28879586E-05        11      .0483222345
        12      3.92271772E-05        12      .0204067877
        13      4.10372863E-05        13      0
        14      1.68339907E-05        14      8.75738963E-03
        H2      .273357907
KG-MOLE FLUORENE/S  IN PRODUCT =  1.09334709E-10
FLUORENE CONVERSION =  86.4425634  %
T-DECALIN CONVERSION=  50.2726748  %
C-DECALIN CONVERSION=  96.4243977  %
```

RUN NUMBER =86 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN86FR
PUMP TEMP/ DEG K =386.483333
INITIAL TIME OF M. B./S =7310.4 FINAL TIME=10922.4
INITIAL PUMP VOL/M3= 1.853E-04 FINAL VOL/M3= 1.935E-04
WT % OF TRANS-DECALIN =30.283
CIS-DECALIN = 46.31
TETRALIN = 1.01
FLUORENE = 22.397
BAROMETRIC PRESSURE/ BARS =1.0256194
P CORRECTION/ BARS = 4.77426E-03
H20 VAPOR PRESS/ BARS = .0352144
WTM SEC/REV AVERAGE=77.7 WTM TEMP/K=299.261111
KGMS OF CATALYST =7.0096E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.0101392 REACTOR TEMP/K=661.205556
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.816667
KGS/SEC IN COND A=1.3927503E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =209
GC AREA COUNTS, GAS 4 =1822 GAS 5 =3642
GC AREA COUNTS, GAS 6 =784 GAS 7 =577

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.08	27	2.738	1	0	27	0
2	.046	28	3.601	2	0	28	0
3	.23	29	31.653	3	0	29	0
4	.358	30	5.215	4	0	30	0
5	.11	31	3.25	5	0	31	0
6	3.911	32	5.113	6	0	32	0
7	.865	33	1.101	7	0	33	0
8	0	34	3.512	8	0	34	0
9	1.13	35	.054	9	0	35	0
10	.972	36	.167	10	0	36	0
11	.218	37	.24	11	0	37	0
12	0	38	.411	12	0	38	0
13	0	39	1.251	13	0	39	0
14	1.645	40	.638	14	0	40	0
15	.125	41	1.088	15	0	41	0
16	.078	42	.812	16	0	42	0
17	.085	43	.409	17	0	43	0
18	.125	44	1.307	18	0	44	0
19	.304	45	0	19	0	45	0
20	.857	46	.37	20	0	46	0
21	.55	47	.233	21	0	47	0
22	1.684	48	7.443	22	0	48	0
23	4.1	49	2.319	23	0	49	0
24	1.574	50	3.253	24	0	50	0
25	1.619	51	0	25	0	51	0
26	3.158	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 86 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	4.32487132E-09	5.9791346E-07
C-DECALIN	6.6137698E-09	9.14353675E-07
TETRALIN	1.50833046E-10	1.9941637E-08
FLUORENE	2.66023424E-09	4.42210737E-07

TOTAL KG-MOLE FED/S = 1.37497084E-08
TOTAL KGS FED/S = 1.97441951E-06
PUMP RATE/ M3/S = 2.27022856E-09
TOTAL KG-ATOMS CARBON= 5.23715843E-04
TOTAL KG-ATOMS HYDROGEN= 8.11101876E-04

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 52.4862591
WHSV (1/S) LIQ FEED BASIS= 2.81671381E-04
VHSV (1/S) = 1.7463157E-04
TOTAL WHSV (1/S) = 4.8757899E-04
MOLAR GAS DENSITY =.272986806 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.82561614
SUPERFICIAL GAS VELOCITY/ M/S = .0137446761

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.39265003E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.43787076E-07
H2 FEEDRATE KG-MOLE/S = 7.21670758E-07
FRACTION OF GAS THAT IS HYDROCARBONS =3.37832043E-03
KG-MOLE/S FREE H2 IN GAS= 7.41274325E-07
H BALANCE CLOSURE = 99.2590788 C BALANCE CLOSURE=77.4260673

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	9.63614053E-04	1	.306971534
	2	3.12486484E-04	2	.0995465507
	3	5.93164725E-05	3	.0188960181
	4	6.46974373E-04	4	.20610193
	5	0	5	0
	6	3.08270256E-04	6	.0982034176
	7	1.15379903E-03	7	0
	8	1.90094523E-04	8	0
	9	4.19665672E-05	9	0
	10	3.48825788E-04	10	.111122899
	11	2.61262479E-04	11	.0832284913
	12	1.47401976E-04	12	.0469567776
	13	2.25641535E-04	13	0
	14	9.09471768E-05	14	.0289723819
	H2	.268236206		

KG-MOLE FLUORENE/S IN PRODUCT = 6.23563387E-10
FLUORENE CONVERSION = 76.5598316 %
T-DECALIN CONVERSION= 26.2743619 %
C-DECALIN CONVERSION= 92.0570453 %

RUN NUMBER =87 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN87FR
PUMP TEMP/ DEG K =388.15
INITIAL TIME OF M. B./S =7318.8 FINAL TIME=11042.4
INITIAL PUMP VOL/M3= 4.088E-05 FINAL VOL/M3= 5.781E-05
WT % OF TRANS-DECALIN =30.365
CIS-DECALIN = 48.394
TETRALIN = 1.068
FLUORENE = 20.173
BAROMETRIC PRESSURE/ BARS =1.0262966
P CORRECTION/ BARS = 4.97742E-03
H20 VAPOR PRESS/ BARS = .0352144
WTM SEC/REV AVERAGE=78.6 WTM TEMP/K=299.538889
KGMS OF CATALYST =7.0002E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=661.261111
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.816667
KGS/SEC IN COND A=3.92245266E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =7E-08
GC AREA COUNTS, GAS 2 =0 GAS 3 =716
GC AREA COUNTS, GAS 4 =5200 GAS 5 =8598
GC AREA COUNTS, GAS 6 =2060 GAS 7 =1274

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.116	27	2.363	1	0	27	0
2	.064	28	4.139	2	0	28	0
3	.21	29	34.371	3	0	29	0
4	.25	30	11.183	4	0	30	0
5	.076	31	2.307	5	0	31	0
6	2.694	32	3.544	6	0	32	0
7	.649	33	.933	7	0	33	0
8	0	34	2.741	8	0	34	0
9	.859	35	.027	9	0	35	0
10	.772	36	.078	10	0	36	0
11	.17	37	.097	11	0	37	0
12	0	38	.188	12	0	38	0
13	0	39	.699	13	0	39	0
14	1.12	40	.281	14	0	40	0
15	.111	41	.458	15	0	41	0
16	.082	42	.339	16	0	42	0
17	.092	43	.094	17	0	43	0
18	.111	44	.332	18	0	44	0
19	.189	45	.081	19	0	45	0
20	.57	46	.598	20	0	46	0
21	.45	47	.324	21	0	47	0
22	1.748	48	8.682	22	0	48	0
23	4.417	49	1.816	23	0	49	0
24	1.291	50	2.773	24	0	50	0
25	1.862	51	0	25	0	51	0
26	3.653	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 87 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	8.62354E-09	1.1922044E-06
C-DECALIN	1.37437047E-08	1.90006718E-06
TETRALIN	3.17164363E-10	4.19323005E-08
FLUORENE	4.76473246E-09	7.92041478E-07

TOTAL KG-MOLE FED/S = 2.74491416E-08
TOTAL KGS FED/S = 3.92624536E-06
PUMP RATE/ M3/S = 4.54671163E-09
TOTAL KG-ATOMS CARBON= 1.03961989E-03
TOTAL KG-ATOMS HYDROGEN= 1.63461625E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 25.9785528
WHSV (1/S) LIQ FEED BASIS= 5.60871683E-04
VHSV (1/S) = 3.49744251E-04
TOTAL WHSV (1/S) = 7.64603939E-04
MOLAR GAS DENSITY =.269202318 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.7258312
SUPERFICIAL GAS VELOCITY/ M/S = .014034892

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 3.92217026E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.21842041E-07
H2 FEEDRATE KG-MOLE/S = 7.13088973E-07
FRACTION OF GAS THAT IS HYDROCARBONS =8.68113748E-03
KG-MOLE/S FREE H2 IN GAS= 7.15575631E-07
H BALANCE CLOSURE = 102.353041 C BALANCE CLOSURE=108.27773

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	2.382811E-03	1	.324178529
	2	6.21282954E-04	2	.0845247878
	3	1.35910179E-04	3	.018490414
	4	1.7139729E-03	4	.233183922
	5	0	5	0
	6	8.78452525E-04	6	.119512394
	7	3.4937852E-03	7	0
	8	1.13674318E-03	8	0
	9	9.91714155E-05	9	0
	10	6.59405564E-04	10	.0897113224
	11	4.43518238E-04	11	.0603401151
	12	2.98757375E-04	12	.0406455764
	13	7.33972097E-04	13	0
	14	2.16194066E-04	14	.0294129389
	H2	.256388341		

KG-MOLE FLUORENE/S IN PRODUCT = 2.04850402E-09
FLUORENE CONVERSION = 57.0069457 %
T-DECALIN CONVERSION= -13.0753365 %
C-DECALIN CONVERSION= 76.9157478 %

RUN NUMBER =88 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN88FR
PUMP TEMP/ DEG K =394.261111
INITIAL TIME OF M. B./S =5484 FINAL TIME=9200.4
INITIAL PUMP VOL/M3= 8.81E-05 FINAL VOL/M3= 1.0922E-04
WT % OF TRANS-DECALIN =30.365
CIS-DECALIN = 48.394
TETRALIN = 1.068
FLUORENE = 20.173
BAROMETRIC PRESSURE/ BARS =1.0273124
P CORRECTION/ BARS = 4.33408E-03
H20 VAPOR PRESS/ BARS = .03714442
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.538889
KGMS OF CATALYST =7.0075E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=15.0101392 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.65
KGS/SEC IN COND A=4.91714334E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =4696
GC AREA COUNTS, GAS 4 =43428 GAS 5 =82838
GC AREA COUNTS, GAS 6 =16624 GAS 7 =13461

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.073	27	1.467	1	0	27	0
2	.032	28	3.292	2	0	28	0
3	.096	29	35.442	3	0	29	0
4	.145	30	16.281	4	0	30	0
5	.045	31	1.673	5	0	31	0
6	1.702	32	2.517	6	0	32	0
7	.221	33	.871	7	0	33	0
8	.024	34	1.923	8	0	34	0
9	.548	35	.022	9	0	35	0
10	.507	36	.079	10	0	36	0
11	.19	37	.121	11	0	37	0
12	0	38	.253	12	0	38	0
13	0	39	.763	13	0	39	0
14	.534	40	.473	14	0	40	0
15	.079	41	1.319	15	0	41	0
16	.048	42	1.297	16	0	42	0
17	.056	43	.168	17	0	43	0
18	.12	44	.062	18	0	44	0
19	.115	45	0	19	0	45	0
20	.286	46	.391	20	0	46	0
21	.303	47	.187	21	0	47	0
22	1.798	48	11.454	22	0	48	0
23	3.718	49	1.829	23	0	49	0
24	.804	50	1.985	24	0	50	0
25	1.654	51	0	25	0	51	0
26	3.116	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 88 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	1.07129052E-08	1.48105914E-06
C-DECALIN	1.70736155E-08	2.36042734E-06
TETRALIN	3.94008929E-10	5.20919205E-08
FLUORENE	5.91916164E-09	9.8394224E-07

TOTAL KG-MOLE FED/S = 3.40996913E-08
TOTAL KGS FED/S = 4.87752065E-06
PUMP RATE/ M3/S = 5.6829644E-09
TOTAL KG-ATOMS CARBON= 1.2915055E-03
TOTAL KG-ATOMS HYDROGEN= 2.0306613E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 21.0669615
WHSV (1/S) LIQ FEED BASIS= 6.96037336E-04
VHSV (1/S) = 4.37147611E-04
TOTAL WHSV (1/S) = 9.01066558E-04
MOLAR GAS DENSITY =.273101507 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.7182173
SUPERFICIAL GAS VELOCITY/ M/S = .0140575405

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 4.91678933E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.21038949E-07
H2 FEEDRATE KG-MOLE/S = 7.18376883E-07
FRACTION OF GAS THAT IS HYDROCARBONS =5.42204597E-03
KG-MOLE/S FREE H2 IN GAS= 7.17129443E-07
H BALANCE CLOSURE = 100.755114 C BALANCE CLOSURE=105.468344

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	1.50508643E-03	1	.234281432
2	5.18572432E-04	2	.0807208738
3	1.17980971E-04	3	.0183648927
4	1.60023659E-03	4	.249092486
5	0	5	0
6	8.77428528E-04	6	.136580337
7	4.54712997E-03	7	0
8	2.08881618E-03	8	0
9	1.16852534E-04	9	0
10	6.19750086E-04	10	.0964701658
11	4.47666246E-04	11	.0696836321
12	5.42215282E-04	12	.0844011148
13	1.22217124E-03	13	0
14	1.95330258E-04	14	.0304050662
H2	.25870227		

KG-MOLE FLUORENE/S IN PRODUCT = 3.38789058E-09
FLUORENE CONVERSION = 42.7640132 %
T-DECALIN CONVERSION= -17.6596142 %
C-DECALIN CONVERSION= 66.0865448 %

RUN NUMBER =89 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN89PR
PUMP TEMP/ DEG K =394.816667
INITIAL TIME OF M. B./S =7806 FINAL TIME=11517
INITIAL PUMP VOL/M3= 1.3427E-04 FINAL VOL/M3= 1.4481E-04
WT % OF TRANS-DECALIN =30.365
CIS-DECALIN = 48.394
TETRALIN = 1.068
FLUORENE = 20.173
BAROMETRIC PRESSURE/ BARS =1.0164772
P CORRECTION/ BARS = 4.16478E-03
H20 VAPOR PRESS/ BARS = .034208758
WTM SEC/REV AVERAGE=78 WTM TEMP/K=298.15
KGMS OF CATALYST =6.9998E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=21.9051392 REACTOR TEMP/K=661.205556
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.261111
KGS/SEC IN COND A=2.35382718E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =3203
GC AREA COUNTS, GAS 4 =27595 GAS 5 =53875
GC AREA COUNTS, GAS 6 =11499 GAS 7 =9080

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.092	27	2.212	1	0	27	0
2	.037	28	4.077	2	0	28	0
3	.088	29	35.516	3	0	29	0
4	.168	30	8.492	4	0	30	0
5	.053	31	2.156	5	0	31	0
6	2.109	32	3.335	6	0	32	0
7	.445	33	1.294	7	0	33	0
8	0	34	2.01	8	0	34	0
9	.694	35	.038	9	0	35	0
10	.657	36	.094	10	0	36	0
11	.135	37	.097	11	0	37	0
12	0	38	.22	12	0	38	0
13	0	39	.539	13	0	39	0
14	.672	40	.27	14	0	40	0
15	.105	41	.636	15	0	41	0
16	.062	42	.682	16	0	42	0
17	.072	43	0	17	0	43	0
18	.135	44	1.03	18	0	44	0
19	.158	45	.873	19	0	45	0
20	.309	46	.32	20	0	46	0
21	.376	47	.165	21	0	47	0
22	3.042	48	9.481	22	0	48	0
23	5.25	49	2.38	23	0	49	0
24	1.03	50	2.05	24	0	50	0
25	2.154	51	0	25	0	51	0
26	4.191	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 89 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.35107614E-09	7.39786277E-07
C-DECALIN	8.52823906E-09	1.17902905E-06
TETRALIN	1.96806724E-10	2.6019817E-08
FLUORENE	2.95661019E-09	4.91477311E-07

TOTAL KG-MOLE FED/S = 1.70327321E-08
TOTAL KGS FED/S = 2.43631245E-06
PUMP RATE/ M3/S = 2.84022752E-09
TOTAL KG-ATOMS CARBON= 6.45104585E-04
TOTAL KG-ATOMS HYDROGEN= 1.01431153E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.040351
WHSV (1/S) LIQ FEED BASIS= 3.48051796E-04
VHSV (1/S) = 2.18477293E-04
TOTAL WHSV (1/S) = 5.52645158E-04
MOLAR GAS DENSITY =.398382675 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =7.06459307
SUPERFICIAL GAS VELOCITY/ M/S = 9.38858474E-03

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.35365772E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.19748976E-07
H2 FEEDRATE KG-MOLE/S = 7.16062036E-07
FRACTION OF GAS THAT IS HYDROCARBONS =3.5392273E-03
KG-MOLE/S FREE H2 IN GAS= 7.1720162E-07
H BALANCE CLOSURE = 100.209097 C BALANCE CLOSURE=102.45163

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	1.45289435E-03	1	.245320653
2	4.48432365E-04	2	.0757176324
3	1.05162935E-04	3	.0177567211
4	1.57202801E-03	4	.265436325
5	0	5	0
6	8.84651491E-04	6	.149373064
7	3.26739625E-03	7	0
8	7.81245888E-04	8	0
9	1.24483809E-04	9	0
10	5.67296678E-04	10	.0957878258
11	4.26709753E-04	11	.0720497777
12	3.20603235E-04	12	.0541337329
13	7.25416852E-04	13	0
14	1.44651015E-04	14	.0244242683
H2	.387561703		

KG-MOLE FLUORENE/S IN PRODUCT = 1.34241887E-09
FLUORENE CONVERSION = 54.5960143 %
T-DECALIN CONVERSION= -12.9954828 %
C-DECALIN CONVERSION= 83.0476939 %

RUN NUMBER =90 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN90PR
PUMP TEMP/ DEG K =390.372222
INITIAL TIME OF M. B./S =8881.2 FINAL TIME=12568.8
INITIAL PUMP VOL/M3= 1.69E-04 FINAL VOL/M3= 1.7946E-04
WT % OF TRANS-DECALIN =30.365
CIS-DECALIN = 48.394
TETRALIN = 1.068
FLUORENE = 20.173
BAROMETRIC PRESSURE/ BARS =1.0154614
P CORRECTION/ BARS = 4.80812E-03
H20 VAPOR PRESS/ BARS = .0402934
WTM SEC/REV AVERAGE=78 WTM TEMP/K=301.761111
KGMS OF CATALYST =7.0009E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=28.8001392 REACTOR TEMP/K=661.483334
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=302.038889
KGS/SEC IN COND A=2.27315406E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =1973
GC AREA COUNTS, GAS 4 =29472 GAS 5 =54044
GC AREA COUNTS, GAS 6 =11840 GAS 7 =9810

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.167	27	2.183	1	0	27	0
2	.07	28	3.666	2	0	28	0
3	.166	29	34.153	3	0	29	0
4	.245	30	10.412	4	0	30	0
5	.081	31	1.984	5	0	31	0
6	2.568	32	2.968	6	0	32	0
7	.381	33	1.25	7	0	33	0
8	0	34	2.054	8	0	34	0
9	.858	35	.047	9	0	35	0
10	.782	36	.116	10	0	36	0
11	.178	37	.123	11	0	37	0
12	.032	38	.285	12	0	38	0
13	0	39	.738	13	0	39	0
14	.85	40	.415	14	0	40	0
15	.122	41	.852	15	0	41	0
16	.076	42	.847	16	0	42	0
17	.078	43	.27	17	0	43	0
18	.138	44	1.045	18	0	44	0
19	.197	45	0	19	0	45	0
20	.429	46	.361	20	0	46	0
21	.398	47	.169	21	0	47	0
22	3.21	48	9.118	22	0	48	0
23	4.737	49	2.04	23	0	49	0
24	1.14	50	2.242	24	0	50	0
25	1.95	51	0	25	0	51	0
26	3.813	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 90 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.36809784E-09	7.42139527E-07
C-DECALIN	8.55536726E-09	1.18277952E-06
TETRALIN	1.97432764E-10	2.61025857E-08
FLUORENE	2.96601512E-09	4.93040694E-07

TOTAL KG-MOLE FED/S = 1.7086913E-08
TOTAL KGS FED/S = 2.44406233E-06
PUMP RATE/ M3/S = 2.83655593E-09
TOTAL KG-ATOMS CARBON= 6.47156654E-04
TOTAL KG-ATOMS HYDROGEN= 1.01753804E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.0780411
WHSV (1/S) LIQ FEED BASIS= 3.49104083E-04
VHSV (1/S) = 2.18194865E-04
TOTAL WHSV (1/S) = 5.49618675E-04
MOLAR GAS DENSITY =.523558654 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =9.46657865
SUPERFICIAL GAS VELOCITY/ M/S = 7.0063888E-03

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.27299041E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.11977084E-07
H2 FEEDRATE KG-MOLE/S = 7.01896914E-07
FRACTION OF GAS THAT IS HYDROCARBONS =3.58726368E-03
KG-MOLE/S FREE H2 IN GAS= 7.09423034E-07
H BALANCE CLOSURE = 100.483086 C BALANCE CLOSURE=98.8087787

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	2.00018118E-03	1	.258409251
2	7.06142354E-04	2	.0912285941
3	1.59105251E-04	3	.0205552723
4	1.99429619E-03	4	.257648951
5	0	5	0
6	1.0473705E-03	6	.135312855
7	4.0327897E-03	7	0
8	1.22945001E-03	8	0
9	1.54343223E-04	9	0
10	6.7519915E-04	10	.0872309511
11	5.33269168E-04	11	.068894602
12	4.21748709E-04	12	.054486948
13	8.95430823E-04	13	0
14	2.03049625E-04	14	.0262325744
H2	.509506278		

KG-MOLE FLUORENE/S IN PRODUCT = 1.24677414E-09
FLUORENE CONVERSION = 57.9646736 %
T-DECALIN CONVERSION= -4.60221902 %
C-DECALIN CONVERSION= 79.9908811 %

RUN NUMBER =91.1 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN91ACT-1
PUMP TEMP/ DEG K =388.705556
INITIAL TIME OF M. B./S =7251 FINAL TIME=10962
INITIAL PUMP VOL/M3= 3.116E-05 FINAL VOL/M3= 4.17E-05
WT % OF TRANS-DECALIN =31.192
CIS-DECALIN = 47.886
TETRALIN = 1.036
FLUORENE = 19.887
BAROMETRIC PRESSURE/ BARS =1.0181702
P CORRECTION/ BARS = 4.19864E-03
H20 VAPOR PRESS/ BARS = .035227944
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.261111
KGMS OF CATALYST =7.0005E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.816667
KGS/SEC IN COND A=1.69733022E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =15582
GC AREA COUNTS, GAS 4 =94109 GAS 5 =127400
GC AREA COUNTS, GAS 6 =41667 GAS 7 =26510

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.147	27	3.639	1	0	27	0
2	.083	28	3.279	2	0	28	0
3	.17	29	33.35	3	0	29	0
4	.24	30	7.808	4	0	30	0
5	.093	31	3.311	5	0	31	0
6	2.138	32	5.459	6	0	32	0
7	.841	33	1.262	7	0	33	0
8	0	34	3.756	8	0	34	0
9	.868	35	.072	9	0	35	0
10	.918	36	.215	10	0	36	0
11	.246	37	.389	11	0	37	0
12	.033	38	.591	12	0	38	0
13	0	39	1.621	13	0	39	0
14	2.9	40	.61	14	0	40	0
15	.139	41	.563	15	0	41	0
16	.094	42	.421	16	0	42	0
17	.072	43	.283	17	0	43	0
18	.034	44	.565	18	0	44	0
19	.677	45	.09	19	0	45	0
20	2.851	46	.643	20	0	46	0
21	1.147	47	.341	21	0	47	0
22	1.583	48	3.1	22	0	48	0
23	3.803	49	1.193	23	0	49	0
24	2.6	50	1.451	24	0	50	0
25	1.453	51	0	25	0	51	0
26	2.862	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 91.1 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.52536113E-09	7.63881177E-07
C-DECALIN	8.48254178E-09	1.1727114E-06
TETRALIN	1.91901353E-10	2.53712779E-08
FLUORENE	2.92983022E-09	4.87025678E-07

TOTAL KG-MOLE FED/S = 1.71296345E-08
TOTAL KGS FED/S = 2.44898954E-06
PUMP RATE/ M3/S = 2.84022751E-09
TOTAL KG-ATOMS CARBON= 6.48303822E-04
TOTAL KG-ATOMS HYDROGEN= 1.02146796E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.6746663
WHSV (1/S) LIQ FEED BASIS= 3.49827861E-04
VHSV (1/S) = 2.18477292E-04
TOTAL WHSV (1/S) = 5.53775034E-04
MOLAR GAS DENSITY =.26933805 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.78989848
SUPERFICIAL GAS VELOCITY/ M/S = .0138471684

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.69720802E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.18886153E-07
H2 FEEDRATE KG-MOLE/S = 7.13871801E-07
FRACTION OF GAS THAT IS HYDROCARBONS =.0104514887
KG-MOLE/S FREE H2 IN GAS= 7.11372722E-07
H BALANCE CLOSURE = 98.132977 C BALANCE CLOSURE=84.6578906

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	2.82793623E-03	1	.507673779
2	2.38439045E-04	2	.0428048023
3	7.01220156E-05	3	.0125883703
4	1.07508813E-03	4	.193000836
5	0	5	0
6	4.01769051E-04	6	.0721259589
7	1.50635164E-03	7	0
8	3.52671473E-04	8	0
9	5.96061013E-05	9	0
10	4.68332098E-04	10	.0840754198
11	3.19200331E-04	11	.0573031443
12	1.19226258E-04	12	.0214036102
13	1.16452269E-04	13	0
14	5.02675601E-05	14	9.02407979E-03
H2	.261732588		

KG-MOLE FLUORENE/S IN PRODUCT = 3.14509948E-10
FLUORENE CONVERSION = 89.1969867 %
T-DECALIN CONVERSION= 25.9022355 %
C-DECALIN CONVERSION= 88.6998624 %

RUN NUMBER =91.2 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN91ACT-2
PUMP TEMP/ DEG K =388.705556
INITIAL TIME OF M. B./S =14697 FINAL TIME=18474
INITIAL PUMP VOL/M3= 5.231E-05 FINAL VOL/M3= 6.286E-05
WT % OF TRANS-DECALIN =31.192
CIS-DECALIN = 47.886
TETRALIN = 1.036
FLUORENE = 19.887
BAROMETRIC PRESSURE/ BARS =1.0181702
P CORRECTION/ BARS = 4.19864E-03
H20 VAPOR PRESS/ BARS = .035227944
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.261111
KGMS OF CATALYST =7.0005E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=661.261111
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.816667
KGS/SEC IN COND A=2.0719713E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =9457
GC AREA COUNTS, GAS 4 =65910 GAS 5 =82555
GC AREA COUNTS, GAS 6 =34163 GAS 7 =25095

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.071	27	2.148	1	0	27	0
2	.047	28	2.55	2	0	28	0
3	.087	29	36.884	3	0	29	0
4	.305	30	21.618	4	0	30	0
5	.126	31	1.812	5	0	31	0
6	2.255	32	2.934	6	0	32	0
7	.899	33	1.025	7	0	33	0
8	.02	34	2.353	8	0	34	0
9	.679	35	.048	9	0	35	0
10	.619	36	.114	10	0	36	0
11	.161	37	.085	11	0	37	0
12	0	38	.2	12	0	38	0
13	0	39	.776	13	0	39	0
14	1.766	40	.294	14	0	40	0
15	.071	41	.501	15	0	41	0
16	.048	42	.292	16	0	42	0
17	.055	43	.102	17	0	43	0
18	.104	44	.301	18	0	44	0
19	.291	45	.057	19	0	45	0
20	.85	46	0	20	0	46	0
21	.4	47	.325	21	0	47	0
22	1.399	48	5.625	22	0	48	0
23	2.441	49	1.284	23	0	49	0
24	1.098	50	1.714	24	0	50	0
25	1.092	51	0	25	0	51	0
26	2.077	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 91.2 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.43396062E-09	7.51245056E-07
C-DECALIN	8.3422236E-09	1.15331241E-06
TETRALIN	1.88726921E-10	2.49515862E-08
FLUORENE	2.88136498E-09	4.78969301E-07

TOTAL KG-MOLE FED/S = 1.68462761E-08
TOTAL KGS FED/S = 2.40847835E-06
PUMP RATE/ M3/S = 2.79324448E-09
TOTAL KG-ATOMS CARBON= 6.37579581E-04
TOTAL KG-ATOMS HYDROGEN= 1.00457084E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.3756441
WHSV (1/S) LIQ FEED BASIS= 3.4404101E-04
VHSV (1/S) = 2.14863241E-04
TOTAL WHSV (1/S) = 5.47988182E-04
MOLAR GAS DENSITY =.269202318 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.78934111
SUPERFICIAL GAS VELOCITY/ M/S = .0138487798

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.07182213E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.06324203E-07
H2 FEEDRATE KG-MOLE/S = 7.13871801E-07
FRACTION OF GAS THAT IS HYDROCARBONS =7.36688222E-03
KG-MOLE/S FREE H2 IN GAS= 7.01120795E-07
H BALANCE CLOSURE = 99.0051335 C BALANCE CLOSURE=96.7082023

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	2.00385832E-03	1	.479293009
2	2.83546732E-04	2	.0678201473
3	5.92110861E-05	3	.0141624083
4	8.06984678E-04	4	.193018693
5	0	5	0
6	3.17450857E-04	6	.0759295079
7	2.06105569E-03	7	0
8	1.20800081E-03	8	0
9	5.98930478E-05	9	0
10	3.00937647E-04	10	.0719797946
11	2.2302403E-04	11	.0533440201
12	1.12389218E-04	12	.0268818238
13	2.61414682E-04	13	0
14	7.34602494E-05	14	.0175705955
H2	.261431091		

KG-MOLE FLUORENE/S IN PRODUCT = 7.0107679E-10
FLUORENE CONVERSION = 75.6685878 %
T-DECALIN CONVERSION= -1.72058613 %
C-DECALIN CONVERSION= 61.1652053 %

RUN NUMBER =91.3 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN91ACT-3
PUMP TEMP/ DEG K =388.705556
INITIAL TIME OF M. B./S =22530 FINAL TIME=26268
INITIAL PUMP VOL/M3= 7.455E-05 FINAL VOL/M3= 8.516E-05
WT % OF TRANS-DECALIN =31.192
CIS-DECALIN = 47.886
TETRALIN = 1.036
FLUORENE = 19.887
BAROMETRIC PRESSURE/ BARS =1.0181702
P CORRECTION/ BARS = 4.19864E-03
H20 VAPOR PRESS/ BARS = .035227944
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.261111
KGMS OF CATALYST =7.0005E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=661.372223
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.261111
KGS/SEC IN COND A=2.18000772E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =1377
GC AREA COUNTS, GAS 4 =48613 GAS 5 =52416
GC AREA COUNTS, GAS 6 =22644 GAS 7 =20354

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.048	27	1.102	1	0	27	0
2	.036	28	0	2	0	28	0
3	.062	29	37.059	3	0	29	0
4	.251	30	33.865	4	0	30	0
5	.097	31	0	5	0	31	0
6	1.736	32	1.543	6	0	32	0
7	.772	33	.826	7	0	33	0
8	.014	34	1.643	8	0	34	0
9	.454	35	.023	9	0	35	0
10	.379	36	.055	10	0	36	0
11	.081	37	.035	11	0	37	0
12	0	38	.104	12	0	38	0
13	0	39	.493	13	0	39	0
14	1.114	40	.188	14	0	40	0
15	.038	41	.419	15	0	41	0
16	.024	42	.248	16	0	42	0
17	.012	43	.083	17	0	43	0
18	.077	44	.248	18	0	44	0
19	.168	45	.122	19	0	45	0
20	.461	46	.703	20	0	46	0
21	.153	47	.398	21	0	47	0
22	.556	48	8.309	22	0	48	0
23	1.175	49	1.294	23	0	49	0
24	.47	50	1.546	24	0	50	0
25	.539	51	0	25	0	51	0
26	.98	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 91.3 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.5218817E-09	7.63400145E-07
C-DECALIN	8.47720016E-09	1.17197292E-06
TETRALIN	1.91780509E-10	2.53553011E-08
FLUORENE	2.92798525E-09	4.86718988E-07

TOTAL KG-MOLE FED/S = 1.71188476E-08
TOTAL KGS FED/S = 2.44744736E-06
PUMP RATE/ M3/S = 2.83843897E-09
TOTAL KG-ATOMS CARBON= 6.47895572E-04
TOTAL KG-ATOMS HYDROGEN= 1.02082473E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.7009262
WHSV (1/S) LIQ FEED BASIS= 3.49607568E-04
VHSV (1/S) = 2.18339713E-04
TOTAL WHSV (1/S) = 5.5355474E-04
MOLAR GAS DENSITY =.269157104 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.78675117
SUPERFICIAL GAS VELOCITY/ M/S = .0138562729

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.17985077E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.15017663E-07
H2 FEEDRATE KG-MOLE/S = 7.13871801E-07
FRACTION OF GAS THAT IS HYDROCARBONS =4.85977786E-03
KG-MOLE/S FREE H2 IN GAS= 7.11542837E-07
H BALANCE CLOSURE = 100.03808 C BALANCE CLOSURE=96.0500778

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	1.33031367E-03	1	.511108452
	2	2.16511392E-04	2	.0831839924
	3	3.58907148E-05	3	.013789265
	4	3.69415979E-04	4	.141930158
	5	0	5	0
	6	1.63482202E-04	6	.0628101005
	7	2.15145132E-03	7	0
	8	1.96602442E-03	8	0
	9	5.01439695E-05	9	0
	10	1.05582904E-04	10	.0405651055
	11	1.64870288E-04	11	.0633434051
	12	1.47894591E-04	12	.0568213176
	13	4.01182816E-04	13	0
	14	6.88394173E-05	14	.0264482045
	H2	.2619855		

KG-MOLE FLUORENE/S IN PRODUCT = 1.08959755E-09
FLUORENE CONVERSION = 62.7867815 %
T-DECALIN CONVERSION= -5.82011308 %
C-DECALIN CONVERSION= 37.0116451 %

RUN NUMBER =91.4 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN91ACT-4
PUMP TEMP/ DEG K =388.705556
INITIAL TIME OF M. B./S =30081.6 FINAL TIME=33821.4
INITIAL PUMP VOL/M3= 9.6E-05 FINAL VOL/M3= 1.066E-04
WT % OF TRANS-DECALIN =31.192
CIS-DECALIN = 47.886
TETRALIN = 1.036
FLUORENE = 19.887
BAROMETRIC PRESSURE/ BARS =1.0181702
P CORRECTION/ BARS = 4.19864E-03
H20 VAPOR PRESS/ BARS = .035227944
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.261111
KGMS OF CATALYST =7.0005E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.261111
KGS/SEC IN COND A=2.19914814E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =609
GC AREA COUNTS, GAS 4 =23532 GAS 5 =22558
GC AREA COUNTS, GAS 6 =10985 GAS 7 =6989

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.035	27	.627	1	0	27	0
2	.031	28	0	2	0	28	0
3	.063	29	34.424	3	0	29	0
4	.242	30	38.54	4	0	30	0
5	.084	31	.914	5	0	31	0
6	1.808	32	.782	6	0	32	0
7	.881	33	0	7	0	33	0
8	0	34	1.261	8	0	34	0
9	.47	35	.018	9	0	35	0
10	.367	36	.036	10	0	36	0
11	.095	37	.024	11	0	37	0
12	0	38	.094	12	0	38	0
13	0	39	.372	13	0	39	0
14	1.122	40	.144	14	0	40	0
15	.028	41	.449	15	0	41	0
16	.017	42	.362	16	0	42	0
17	.018	43	.529	17	0	43	0
18	.075	44	0	18	0	44	0
19	.131	45	0	19	0	45	0
20	.372	46	.241	20	0	46	0
21	.11	47	.128	21	0	47	0
22	.305	48	10.494	22	0	48	0
23	.659	49	1.286	23	0	49	0
24	.269	50	1.273	24	0	50	0
25	.291	51	0	25	0	51	0
26	.531	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 91.4 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.51402206E-09	7.6231355E-07
C-DECALIN	8.46513402E-09	1.17030478E-06
TETRALIN	1.91507535E-10	2.53192113E-08
FLUORENE	2.92381766E-09	4.86026211E-07

TOTAL KG-MOLE FED/S = 1.70944813E-08
TOTAL KGS FED/S = 2.44396375E-06
PUMP RATE/ M3/S = 2.83439884E-09
TOTAL KG-ATOMS CARBON= 6.46973381E-04
TOTAL KG-ATOMS HYDROGEN= 1.01937172E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.7603664
WHSV (1/S) LIQ FEED BASIS= 3.49109949E-04
VHSV (1/S) = 2.18028936E-04
TOTAL WHSV (1/S) = 5.53057122E-04
MOLAR GAS DENSITY =.26933805 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.79012883
SUPERFICIAL GAS VELOCITY/ M/S = .0138465025

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.19898981E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.14673518E-07
H2 FEEDRATE KG-MOLE/S = 7.13871801E-07
FRACTION OF GAS THAT IS HYDROCARBONS =2.18522883E-03
KG-MOLE/S FREE H2 IN GAS= 7.13111793E-07
H BALANCE CLOSURE = 99.2997461 C BALANCE CLOSURE=93.0242099

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	6.2254275E-04	1	.362499187
	2	2.27395654E-04	2	.132409766
	3	3.36152128E-05	3	.0195737358
	4	3.11393957E-04	4	.181320972
	5	0	5	0
	6	9.24505882E-05	6	.0538328702
	7	2.01808437E-03	7	0
	8	2.25938216E-03	8	0
	9	0	9	0
	10	1.13503617E-04	10	.0660917964
	11	1.38456518E-04	11	.0806215719
	12	1.20765311E-04	12	.0703201942
	13	5.11652123E-04	13	0
	14	5.72395559E-05	14	.0333299078
	H2	.262831568		

KG-MOLE FLUORENE/S IN PRODUCT = 1.38820905E-09
FLUORENE CONVERSION = 52.5206695 %
T-DECALIN CONVERSION= .699619749 %
C-DECALIN CONVERSION= 27.5837637 %

RUN NUMBER =91.5 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN91ACT-5
PUMP TEMP/ DEG K =388.705556
INITIAL TIME OF M. B./S =37815 FINAL TIME=42013.2
INITIAL PUMP VOL/M3= 1.179E-04 FINAL VOL/M3= 1.2986E-04
WT % OF TRANS-DECALIN =31.192
CIS-DECALIN = 47.886
TETRALIN = 1.036
FLUORENE = 19.887
BAROMETRIC PRESSURE/ BARS =1.0181702
P CORRECTION/ BARS = 4.19864E-03
H20 VAPOR PRESS/ BARS = .035227944
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.261111
KGMS OF CATALYST =7.0005E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .076464
WTM TEMP/DEG K DURING M.B.=299.261111
KGS/SEC IN COND A=2.28304374E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =955
GC AREA COUNTS, GAS 4 =23094 GAS 5 =19860
GC AREA COUNTS, GAS 6 =11651 GAS 7 =5052

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.026	27	.524	1	0	27	0
2	.025	28	0	2	0	28	0
3	.029	29	33.633	3	0	29	0
4	.113	30	41.717	4	0	30	0
5	.038	31	.592	5	0	31	0
6	.985	32	.813	6	0	32	0
7	.584	33	0	7	0	33	0
8	.011	34	1.036	8	0	34	0
9	.294	35	9E-03	9	0	35	0
10	.233	36	.019	10	0	36	0
11	.049	37	7E-03	11	0	37	0
12	0	38	.045	12	0	38	0
13	0	39	.289	13	0	39	0
14	.822	40	.116	14	0	40	0
15	0	41	.262	15	0	41	0
16	0	42	.14	16	0	42	0
17	0	43	.093	17	0	43	0
18	.067	44	.032	18	0	44	0
19	.097	45	0	19	0	45	0
20	.285	46	.285	20	0	46	0
21	.077	47	.121	21	0	47	0
22	.246	48	12.314	22	0	48	0
23	.477	49	1.44	23	0	49	0
24	.214	50	1.229	24	0	50	0
25	.223	51	0	25	0	51	0
26	.392	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 91.5 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.5421601E-09	7.66203634E-07
C-DECALIN	8.50833158E-09	1.17627684E-06
TETRALIN	1.92484798E-10	2.54484151E-08
FLUORENE	2.9387379E-09	4.88506401E-07

TOTAL KG-MOLE FED/S = 1.71817144E-08
TOTAL KGS FED/S = 2.45643529E-06
PUMP RATE/ M3/S = 2.84886277E-09
TOTAL KG-ATOMS CARBON= 6.50274885E-04
TOTAL KG-ATOMS HYDROGEN= 1.02457357E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.5483453
WHSV (1/S) LIQ FEED BASIS= 3.50891456E-04
VHSV (1/S) = 2.19141537E-04
TOTAL WHSV (1/S) = 5.54838629E-04
MOLAR GAS DENSITY =.26933805 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.78955724
SUPERFICIAL GAS VELOCITY/ M/S = .0138481549

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.28287937E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.16218385E-07
H2 FEEDRATE KG-MOLE/S = 7.13871801E-07
FRACTION OF GAS THAT IS HYDROCARBONS =2.06927125E-03
KG-MOLE/S FREE H2 IN GAS= 7.14736335E-07
H BALANCE CLOSURE = 99.8813867 C BALANCE CLOSURE=95.7659492

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	5.70264241E-04	1	.40890964
2	1.32547911E-04	2	.0950438668
3	2.10111809E-05	3	.0150661286
4	2.33370056E-04	4	.167338681
5	0	5	0
6	7.43006237E-05	6	.0532774793
7	2.04162817E-03	7	0
8	2.53235222E-03	8	0
9	0	9	0
10	9.37761222E-05	10	.0672424424
11	9.87818603E-05	11	.0708318215
12	1.13324559E-04	12	.0812597058
13	6.21678611E-04	13	0
14	5.72206505E-05	14	.0410302346
H2	.262747794		

KG-MOLE FLUORENE/S IN PRODUCT = 1.69111331E-09
FLUORENE CONVERSION = 42.4544355 %
T-DECALIN CONVERSION= -.208454501 %
C-DECALIN CONVERSION= 19.0370196 %

RUN NUMBER =91.6 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN91ACT-6
PUMP TEMP/ DEG K =388.705556
INITIAL TIME OF M. B./S =48867.6 FINAL TIME=52592.4
INITIAL PUMP VOL/M3= 1.493E-04 FINAL VOL/M3= 1.5988E-04
WT % OF TRANS-DECALIN =31.192
CIS-DECALIN = 47.886
TETRALIN = 1.036
FLUORENE = 19.887
BAROMETRIC PRESSURE/ BARS =1.0181702
P CORRECTION/ BARS = 4.19864E-03
H20 VAPOR PRESS/ BARS = .035227944
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.261111
KGMS OF CATALYST =7.0005E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.816667
KGS/SEC IN COND A=2.23473432E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =718
GC AREA COUNTS, GAS 4 =18235 GAS 5 =14509
GC AREA COUNTS, GAS 6 =10120 GAS 7 =10261

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.012	27	.291	1	0	27	0
2	.019	28	0	2	0	28	0
3	.023	29	33.401	3	0	29	0
4	.013	30	45.016	4	0	30	0
5	.036	31	.359	5	0	31	0
6	.449	32	.895	6	0	32	0
7	.346	33	0	7	0	33	0
8	0	34	.808	8	0	34	0
9	.131	35	.019	9	0	35	0
10	.13	36	.039	10	0	36	0
11	0	37	0	11	0	37	0
12	0	38	0	12	0	38	0
13	0	39	.215	13	0	39	0
14	.568	40	.081	14	0	40	0
15	0	41	.182	15	0	41	0
16	0	42	.083	16	0	42	0
17	0	43	.051	17	0	43	0
18	.058	44	.032	18	0	44	0
19	.07	45	0	19	0	45	0
20	.212	46	.195	20	0	46	0
21	.052	47	.096	21	0	47	0
22	.087	48	13.719	22	0	48	0
23	.036	49	1.017	23	0	49	0
24	.223	50	.72	24	0	50	0
25	.132	51	0	25	0	51	0
26	.183	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 91.6 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.52578164E-09	7.63939312E-07
C-DECALIN	8.48318734E-09	1.17280065E-06
TETRALIN	1.91915958E-10	2.53732088E-08
FLUORENE	2.9300532E-09	4.87062743E-07

TOTAL KG-MOLE FED/S = 1.71309381E-08
TOTAL KGS FED/S = 2.44917591E-06
PUMP RATE/ M3/S = 2.84044367E-09
TOTAL KG-ATOMS CARBON= 6.48353161E-04
TOTAL KG-ATOMS HYDROGEN= 1.0215457E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.6714949
WHSV (1/S) LIQ FEED BASIS= 3.49854485E-04
VHSV (1/S) = 2.18493919E-04
TOTAL WHSV (1/S) = 5.53801658E-04
MOLAR GAS DENSITY =.26933805 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.78988993
SUPERFICIAL GAS VELOCITY/ M/S = .0138471931

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.23457343E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.16222752E-07
H2 FEEDRATE KG-MOLE/S = 7.13871801E-07
FRACTION OF GAS THAT IS HYDROCARBONS =1.78852761E-03
KG-MOLE/S FREE H2 IN GAS= 7.14941767E-07
H BALANCE CLOSURE = 99.5725889 C BALANCE CLOSURE=93.7339

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	4.82912568E-04	1	.48679564
2	5.90716485E-05	2	.0595466403
3	1.08833846E-05	3	.0109708973
4	1.46655845E-04	4	.147835096
5	0	5	0
6	2.72920043E-05	6	.0275114578
7	1.98601359E-03	7	0
8	2.67663806E-03	8	0
9	0	9	0
10	8.1229758E-05	10	.0818829219
11	7.34756339E-05	11	.0740664473
12	7.76667435E-05	12	.0782912574
13	6.78423585E-04	13	0
14	3.28356116E-05	14	.0330996408
H2	.263004952		

KG-MOLE FLUORENE/S IN PRODUCT = 1.84419857E-09
FLUORENE CONVERSION = 37.059212 %
T-DECALIN CONVERSION= 2.29984766 %
C-DECALIN CONVERSION= 14.2296199 %

RUN NUMBER =91.7 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN91ACT-7
PUMP TEMP/ DEG K =388.705556
INITIAL TIME OF M. B./S =60526.8 FINAL TIME=64242
INITIAL PUMP VOL/M3= 1.824E-04 FINAL VOL/M3= 1.9296E-04
WT % OF TRANS-DECALIN =31.192
CIS-DECALIN = 47.886
TETRALIN = 1.036
FLUORENE = 19.887
BAROMETRIC PRESSURE/ BARS =1.0181702
P CORRECTION/ BARS = 4.19864E-03
H20 VAPOR PRESS/ BARS = .035227944
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.261111
KGMS OF CATALYST =7.0005E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.372223
KGS/SEC IN COND A=2.49953328E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =975
GC AREA COUNTS, GAS 4 =18736 GAS 5 =13646
GC AREA COUNTS, GAS 6 =11002 GAS 7 =4241

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.014	27	.218	1	0	27	0
2	.018	28	0	2	0	28	0
3	8E-03	29	32.583	3	0	29	0
4	.013	30	45.652	4	0	30	0
5	0	31	.231	5	0	31	0
6	.221	32	.941	6	0	32	0
7	.217	33	0	7	0	33	0
8	.082	34	.639	8	0	34	0
9	0	35	0	9	0	35	0
10	.073	36	0	10	0	36	0
11	0	37	0	11	0	37	0
12	0	38	.04	12	0	38	0
13	0	39	.17	13	0	39	0
14	.399	40	.061	14	0	40	0
15	0	41	.142	15	0	41	0
16	0	42	.064	16	0	42	0
17	0	43	.036	17	0	43	0
18	.062	44	.017	18	0	44	0
19	.049	45	0	19	0	45	0
20	.151	46	.173	20	0	46	0
21	.037	47	0	21	0	47	0
22	.097	48	15.602	22	0	48	0
23	.053	49	.937	23	0	49	0
24	.164	50	.595	24	0	50	0
25	.112	51	0	25	0	51	0
26	.132	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 91.7 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.52958748E-09	7.64465469E-07
C-DECALIN	8.48903008E-09	1.17360841E-06
TETRALIN	1.92048138E-10	2.53906844E-08
FLUORENE	2.93207125E-09	4.87398204E-07

TOTAL KG-MOLE FED/S = 1.7142737E-08
TOTAL KGS FED/S = 2.45086277E-06
PUMP RATE/ M3/S = 2.8424E-09
TOTAL KG-ATOMS CARBON= 6.4879971E-04
TOTAL KG-ATOMS HYDROGEN= 1.02224928E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.6428137
WHSV (1/S) LIQ FEED BASIS= 3.50095445E-04
VHSV (1/S) = 2.18644405E-04
TOTAL WHSV (1/S) = 5.54042617E-04
MOLAR GAS DENSITY =.26933805 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.78981262
SUPERFICIAL GAS VELOCITY/ M/S = .0138474166

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.49935333E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.16746152E-07
H2 FEEDRATE KG-MOLE/S = 7.13871801E-07
FRACTION OF GAS THAT IS HYDROCARBONS =1.66278198E-03
KG-MOLE/S FREE H2 IN GAS= 7.15554359E-07
H BALANCE CLOSURE = 101.273353 C BALANCE CLOSURE=104.264203

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	4.44502484E-04	1	.504774765
2	2.91326211E-05	2	.0330828567
3	1.57447711E-05	3	.0178796821
4	1.15577429E-04	4	.131249142
5	0	5	0
6	2.53921585E-05	6	.0288352063
7	2.16018982E-03	7	0
8	3.02663921E-03	8	0
9	0	9	0
10	8.3758654E-05	10	.0951159025
11	6.38323893E-05	11	.0724877374
12	7.23994524E-05	12	.0822164508
13	8.60274113E-04	13	0
14	3.02557329E-05	14	.0343582568
H2	.262410351		

KG-MOLE FLUORENE/S IN PRODUCT = 2.34584074E-09
FLUORENE CONVERSION = 19.9937335 %
T-DECALIN CONVERSION= -6.52728308 %
C-DECALIN CONVERSION= 2.77806697 %

RUN NUMBER =92 . INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN92ACT
PUMP TEMP/ DEG K =389.261111
INITIAL TIME OF M. B./S =25381.2 FINAL TIME=29028
INITIAL PUMP VOL/M3= 8.555E-05 FINAL VOL/M3= 9.591E-05
WT % OF TRANS-DECALIN =31.37
CIS-DECALIN = 48.129
TETRALIN = 1.042
FLUORENE = 19.369
BAROMETRIC PRESSURE/ BARS =1.0171544
P CORRECTION/ BARS = 4.33408E-03
H20 VAPOR PRESS/ BARS = .03822794
WTM SEC/REV AVERAGE=77.4 WTM TEMP/K=299.816667
KGMS OF CATALYST =7.0082E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.65
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=301.205556
KGS/SEC IN COND A=2.34260406E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =1162
GC AREA COUNTS, GAS 4 =28709 GAS 5 =35318
GC AREA COUNTS, GAS 6 =11582 GAS 7 =7646

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.051	27	1.145	1	0	27	0
2	.03	28	1.728	2	0	28	0
3	.034	29	37.851	3	0	29	0
4	.05	30	29.296	4	0	30	0
5	.016	31	1.162	5	0	31	0
6	.628	32	2.021	6	0	32	0
7	.306	33	.831	7	0	33	0
8	0	34	1.836	8	0	34	0
9	.279	35	.021	9	0	35	0
10	.269	36	.049	10	0	36	0
11	.056	37	.028	11	0	37	0
12	0	38	.094	12	0	38	0
13	0	39	.483	13	0	39	0
14	.583	40	.181	14	0	40	0
15	.035	41	.41	15	0	41	0
16	.02	42	.249	16	0	42	0
17	.019	43	.058	17	0	43	0
18	.085	44	.2	18	0	44	0
19	.124	45	.051	19	0	45	0
20	.338	46	.511	20	0	46	0
21	.143	47	.204	21	0	47	0
22	.771	48	9.956	22	0	48	0
23	1.642	49	1.555	23	0	49	0
24	.546	50	1.867	24	0	50	0
25	.759	51	0	25	0	51	0
26	1.43	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 92 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.55307187E-09	7.67712187E-07
C-DECALIN	8.51972573E-09	1.17785208E-06
TETRALIN	1.92880059E-10	2.55006726E-08
FLUORENE	2.85155472E-09	4.74013941E-07

TOTAL KG-MOLE FED/S = 1.71172324E-08
TOTAL KGS FED/S = 2.44507888E-06
PUMP RATE/ M3/S = 2.8408695E-09
TOTAL KG-ATOMS CARBON= 6.47011981E-04
TOTAL KG-ATOMS HYDROGEN= 1.02289749E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.772397
WHSV (1/S) LIQ FEED BASIS= 3.48885495E-04
VHSV (1/S) = 2.18526675E-04
TOTAL WHSV (1/S) = 5.52938491E-04
MOLAR GAS DENSITY =.269451265 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.78442683
SUPERFICIAL GAS VELOCITY/ M/S = .0138630045

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.34243541E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.2508215E-07
H2 FEEDRATE KG-MOLE/S = 7.15027826E-07
FRACTION OF GAS THAT IS HYDROCARBONS =2.85445743E-03
KG-MOLE/S FREE H2 IN GAS= 7.23012433E-07
H BALANCE CLOSURE = 101.203895 C BALANCE CLOSURE=100.130581

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	7.73964534E-04	1	.351013377
2	1.00453412E-04	2	.0455582781
3	2.7396733E-05	3	.0124251427
4	4.52317243E-04	4	.205137827
5	0	5	0
6	2.18177895E-04	6	.0989494431
7	2.32889213E-03	7	0
8	1.80252104E-03	8	0
9	5.34655298E-05	9	0
10	2.1596056E-04	10	.0979438229
11	1.78590106E-04	11	.0809953341
12	1.49976503E-04	12	.0680183087
13	5.09462988E-04	13	0
14	8.81061452E-05	14	.039958466
H2	.26255198		

KG-MOLE FLUORENE/S IN PRODUCT = 1.40295295E-09
FLUORENE CONVERSION = 50.8004199 %
T-DECALIN CONVERSION= -15.4905758 %
C-DECALIN CONVERSION= 41.7380258 %

RUN NUMBER =93 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN93TP
PUMP TEMP/ DEG K =393.705556
INITIAL TIME OF M. B./S =8439 FINAL TIME=12136.2
INITIAL PUMP VOL/M3= 1.1792E-04 FINAL VOL/M3= 1.2843E-04
WT % OF TRANS-DECALIN =31.37
CIS-DECALIN = 48.219
TETRALIN = 1.042
FLUORENE = 19.369
BAROMETRIC PRESSURE/ BARS =1.0218948
P CORRECTION/ BARS = 4.36794E-03
H20 VAPOR PRESS/ BARS = .03778776
WTM SEC/REV AVERAGE=78 WTM TEMP/K=298.705556
KGMS OF CATALYST =7.0044E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.927778
KGS/SEC IN COND A=2.20520418E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =18358 GAS 5 =41869
GC AREA COUNTS, GAS 6 =6606 GAS 7 =6718

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.011	27	1.773	1	0	27	0
2	.056	28	3.693	2	0	28	0
3	.08	29	37.096	3	0	29	0
4	.208	30	11.658	4	0	30	0
5	.069	31	2.276	5	0	31	0
6	2.07	32	3.58	6	0	32	0
7	.368	33	1.1	7	0	33	0
8	0	34	2.173	8	0	34	0
9	.578	35	.019	9	0	35	0
10	.533	36	.055	10	0	36	0
11	.103	37	.059	11	0	37	0
12	0	38	.118	12	0	38	0
13	0	39	.374	13	0	39	0
14	.529	40	.146	14	0	40	0
15	.081	41	.323	15	0	41	0
16	.041	42	.339	16	0	42	0
17	.051	43	.055	17	0	43	0
18	.127	44	.281	18	0	44	0
19	.124	45	.083	19	0	45	0
20	.257	46	.395	20	0	46	0
21	.331	47	.15	21	0	47	0
22	2.502	48	10.879	22	0	48	0
23	4.383	49	2.399	23	0	49	0
24	.873	50	1.895	24	0	50	0
25	1.936	51	0	25	0	51	0
26	3.765	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 93 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.52689925E-09	7.64093821E-07
C-DECALIN	8.49542731E-09	1.17449283E-06
TETRALIN	1.9197098E-10	2.53804833E-08
FLUORENE	2.83811483E-09	4.71779828E-07

TOTAL KG-MOLE FED/S = 1.70524124E-08
TOTAL KGS FED/S = 2.43574696E-06
PUMP RATE/ M3/S = 2.84271451E-09
TOTAL KG-ATOMS CARBON= 6.44533329E-04
TOTAL KG-ATOMS HYDROGEN= 1.01910389E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.9838622
WHSV (1/S) LIQ FEED BASIS= 3.47742486E-04
VHSV (1/S) = 2.18668598E-04
TOTAL WHSV (1/S) = 5.5216268E-04
MOLAR GAS DENSITY =.26933805 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.77697839
SUPERFICIAL GAS VELOCITY/ M/S = .0138846202

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.20504542E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.19638018E-07
H2 FEEDRATE KG-MOLE/S = 7.15926131E-07
FRACTION OF GAS THAT IS HYDROCARBONS =2.42950631E-03
KG-MOLE/S FREE H2 IN GAS= 7.17889653E-07
H BALANCE CLOSURE = 98.9705232 C BALANCE CLOSURE=94.7609944

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	6.84062087E-04	1	.21642185
2	2.66544461E-04	2	.0843286691
3	5.32991455E-05	3	.0168626502
4	8.65841038E-04	4	.273932619
5	0	5	0
6	4.72356863E-04	6	.149443081
7	2.16541648E-03	7	0
8	6.80516103E-04	8	0
9	6.71441028E-05	9	0
10	3.71304818E-04	10	.117472488
11	1.88148496E-04	11	.0595259502
12	1.74381666E-04	12	.055170435
13	5.28152168E-04	13	0
14	8.48424959E-05	14	.0268422564
H2	.26273604		

KG-MOLE FLUORENE/S IN PRODUCT = 1.44310227E-09
FLUORENE CONVERSION = 49.1527877 %
T-DECALIN CONVERSION= -7.0527762 %
C-DECALIN CONVERSION= 78.1127488 %

RUN NUMBER =94 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN94TP
PUMP TEMP/ DEG K =394.261111
INITIAL TIME OF M. B./S =8573.4 FINAL TIME=12302.4
INITIAL PUMP VOL/M3= 1.5232E-04 FINAL VOL/M3= 1.6292E-04
WT % OF TRANS-DECALIN =31.37
CIS-DECALIN = 48.219
TETRALIN = 1.042
FLUORENE = 19.369
BAROMETRIC PRESSURE/ BARS =1.0181702
P CORRECTION/ BARS = 4.7404E-03
H20 VAPOR PRESS/ BARS = .03778776
WTM SEC/REV AVERAGE=78 WTM TEMP/K=300.372223
KGMS OF CATALYST =7.0077E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.761112
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.927778
KGS/SEC IN COND A=1.85648184E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =4373
GC AREA COUNTS, GAS 4 =35685 GAS 5 =59762
GC AREA COUNTS, GAS 6 =14357 GAS 7 =7680

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.026	27	3.364	1	0	27	0
2	.095	28	3.775	2	0	28	0
3	.073	29	30.667	3	0	29	0
4	.112	30	5.608	4	0	30	0
5	.039	31	3.354	5	0	31	0
6	1.447	32	5.275	6	0	32	0
7	.407	33	1.114	7	0	33	0
8	0	34	3.811	8	0	34	0
9	.62	35	.126	9	0	35	0
10	.66	36	.27	10	0	36	0
11	.16	37	.35	11	0	37	0
12	.026	38	.511	12	0	38	0
13	0	39	1.456	13	0	39	0
14	1.198	40	.689	14	0	40	0
15	.122	41	.738	15	0	41	0
16	.087	42	.683	16	0	42	0
17	.1	43	.365	17	0	43	0
18	.202	44	.877	18	0	44	0
19	.359	45	.394	19	0	45	0
20	1.092	46	1.23	20	0	46	0
21	.833	47	.742	21	0	47	0
22	3.183	48	6.229	22	0	48	0
23	5.093	49	1.753	23	0	49	0
24	1.924	50	3.253	24	0	50	0
25	1.923	51	0	25	0	51	0
26	3.585	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 94 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.5236003E-09	7.6363774E-07
C-DECALIN	8.49035648E-09	1.17379178E-06
TETRALIN	1.91856395E-10	2.53653339E-08
FLUORENE	2.83642079E-09	4.71498227E-07

TOTAL KG-MOLE FED/S = 1.7042234E-08
TOTAL KGS FED/S = 2.43429308E-06
PUMP RATE/ M3/S = 2.84260787E-09
TOTAL KG-ATOMS CARBON= 6.44148614E-04
TOTAL KG-ATOMS HYDROGEN= 1.0184956E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.6012871
WHSV (1/S) LIQ FEED BASIS= 3.47371265E-04
VHSV (1/S) = 2.18660395E-04
TOTAL WHSV (1/S) = 5.4971246E-04
MOLAR GAS DENSITY =.269405968 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.82397218
SUPERFICIAL GAS VELOCITY/ M/S = .0137493601

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.85634818E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.10517412E-07
H2 FEEDRATE KG-MOLE/S = 7.08978867E-07
FRACTION OF GAS THAT IS HYDROCARBONS =4.14769771E-03
KG-MOLE/S FREE H2 IN GAS= 7.07570401E-07
H BALANCE CLOSURE = 96.4681003 C BALANCE CLOSURE=83.0510975

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	1.1294868E-03	1	.273980395
2	1.92927141E-04	2	.04679847
3	6.00643398E-05	3	.0145698485
4	9.90384401E-04	4	.240238229
5	0	5	0
6	5.18362659E-04	6	.125739589
7	1.53146702E-03	7	0
8	2.80055664E-04	8	0
9	5.81731232E-05	9	0
10	5.0996204E-04	10	.123701845
11	3.82794326E-04	11	.0928546844
12	2.13930095E-04	12	.051893171
13	2.58708335E-04	13	0
14	1.24597774E-04	14	.0302237683
H2	.263155054		

KG-MOLE FLUORENE/S IN PRODUCT = 6.95614079E-10
FLUORENE CONVERSION = 75.4756388 %
T-DECALIN CONVERSION= 25.4507383 %
C-DECALIN CONVERSION= 91.1309648 %

RUN NUMBER =95 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN95TP
PUMP TEMP/ DEG K =394.816667
INITIAL TIME OF M. B./S =11046 FINAL TIME=14726.4
INITIAL PUMP VOL/M3= 1.936E-04 FINAL VOL/M3= 2.0406E-04
WT % OF TRANS-DECALIN =31.37
CIS-DECALIN = 48.219
TETRALIN = 1.042
FLUORENE = 19.369
BAROMETRIC PRESSURE/ BARS =1.0117368
P CORRECTION/ BARS = 4.97742E-03
H20 VAPOR PRESS/ BARS = .037246
WTM SEC/REV AVERAGE=77.7 WTM TEMP/K=300.094445
KGMS OF CATALYST =7.0049E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=661.483334
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.65
KGS/SEC IN COND A=1.89670728E-06 KGS/SEC IN B = 3.366E-07
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =6333
GC AREA COUNTS, GAS 4 =46211 GAS 5 =72704
GC AREA COUNTS, GAS 6 =19101 GAS 7 =11767

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.026	27	2.813	1	.25	27	.528
2	.088	28	3.644	2	.283	28	.638
3	.059	29	35.792	3	2.25	29	3.794
4	.094	30	7.991	4	3.742	30	1.327
5	.031	31	2.667	5	1.192	31	.164
6	1.226	32	4.232	6	34.242	32	.238
7	.373	33	.982	7	5.606	33	0
8	0	34	3.161	8	2.074	34	.145
9	.536	35	.05	9	9.506	35	0
10	.56	36	.143	10	7.155	36	0
11	.13	37	.186	11	1.579	37	0
12	0	38	.339	12	.236	38	0
13	0	39	1.258	13	.051	39	0
14	.961	40	.637	14	12.509	40	0
15	.093	41	1.155	15	.674	41	0
16	.06	42	.816	16	.412	42	0
17	.067	43	.441	17	.275	43	0
18	.128	44	1.052	18	.289	44	0
19	.253	45	.311	19	1.106	45	0
20	.72	46	.478	20	4.928	46	0
21	.528	47	.269	21	1.407	47	0
22	1.79	48	7.546	22	.728	48	0
23	4.508	49	1.855	23	1.07	49	0
24	1.558	50	3.106	24	.698	50	0
25	1.821	51	0	25	.316	51	0
26	3.467	52	0	26	.587	52	0
		53	0			53	0

RUN NUMBER 95 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.51952786E-09	7.63074726E-07
C-DECALIN	8.48409671E-09	1.17292637E-06
TETRALIN	1.91714943E-10	2.53466326E-08
FLUORENE	2.83432955E-09	4.71150602E-07

TOTAL KG-MOLE FED/S = 1.70296691E-08
TOTAL KGS FED/S = 2.43249833E-06
PUMP RATE/ M3/S = 2.84210511E-09
TOTAL KG-ATOMS CARBON= 6.43673697E-04
TOTAL KG-ATOMS HYDROGEN= 1.01774468E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.568613
WHSV (1/S) LIQ FEED BASIS= 3.47253904E-04
VHSV (1/S) = 2.18621722E-04
TOTAL WHSV (1/S) = 5.4936787E-04
MOLAR GAS DENSITY =.269111906 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.82596347
SUPERFICIAL GAS VELOCITY/ M/S = .0137436868

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.89657073E-06 KGS/S,COND B= 3.36558248E-07
KG-MOLE/S OF ALL GAS OUT= 7.16038236E-07
H2 FEEDRATE KG-MOLE/S = 7.07899723E-07
FRACTION OF GAS THAT IS HYDROCARBONS =5.31733722E-03
KG-MOLE/S FREE H2 IN GAS= 7.1223082E-07
H BALANCE CLOSURE = 100.602721 C BALANCE CLOSURE=100.008189
PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	1.54642909E-03	1	.294138902
2	8.12666502E-04	2	.154573419
3	1.80406525E-04	3	.0343142648
4	1.17936373E-03	4	.22432115
5	0	5	0
6	4.7709381E-04	6	.0907457381
7	1.83484434E-03	7	0
8	4.13936845E-04	8	0
9	5.16692467E-05	9	0
10	4.00914785E-04	10	.0762560892
11	3.47304511E-04	11	.0660591347
12	1.93429848E-04	12	.0367913689
13	3.15785616E-04	13	0
14	1.19870171E-04	14	.0227999336
H2	.261238191		

KG-MOLE FLUORENE/S IN PRODUCT = 8.60947043E-10
FLUORENE CONVERSION = 69.6243141 %
T-DECALIN CONVERSION= 9.36803562 %
C-DECALIN CONVERSION= 86.698134 %

RUN NUMBER =96 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN96TP
PUMP TEMP/ DEG K =385.927778
INITIAL TIME OF M. B./S =9704.4 FINAL TIME=13397.4
INITIAL PUMP VOL/M3= 3.554E-05 FINAL VOL/M3= 4.603E-05
WT % OF TRANS-DECALIN =30.575
CIS-DECALIN = 47.477
TETRALIN = 1.03
FLUORENE = 20.92
BAROMETRIC PRESSURE/ BARS =1.0249422
P CORRECTION/ BARS = 4.4018E-03
H20 VAPOR PRESS/ BARS = .03822794
WTM SEC/REV AVERAGE=77.4 WTM TEMP/K=300.927778
KGMS OF CATALYST =7.0444E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=677.872223
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=301.205556
KGS/SEC IN COND A=2.11355796E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =2228
GC AREA COUNTS, GAS 4 =41420 GAS 5 =61173
GC AREA COUNTS, GAS 6 =17085 GAS 7 =17888

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.081	27	1.99	1	0	27	0
2	.045	28	2.895	2	0	28	0
3	.089	29	34.028	3	0	29	0
4	.172	30	13.418	4	0	30	0
5	.056	31	2.251	5	0	31	0
6	1.821	32	3.757	6	0	32	0
7	.57	33	.674	7	0	33	0
8	0	34	3.39	8	0	34	0
9	.659	35	.029	9	0	35	0
10	.624	36	.113	10	0	36	0
11	.149	37	.142	11	0	37	0
12	0	38	.219	12	0	38	0
13	0	39	1.154	13	0	39	0
14	1.444	40	.432	14	0	40	0
15	.084	41	.699	15	0	41	0
16	.069	42	.702	16	0	42	0
17	.061	43	.441	17	0	43	0
18	.101	44	1.375	18	0	44	0
19	.249	45	0	19	0	45	0
20	.847	46	.463	20	0	46	0
21	.371	47	.286	21	0	47	0
22	1.[illegible]6	48	9.57	22	0	48	0
23	2.975	49	1.89	23	0	49	0
24	1.199	50	3.337	24	0	50	0
25	1.266	51	0	25	0	51	0
26	2.4	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 96 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.4461271E-09	7.52927071E-07
C-DECALIN	8.4567711E-09	1.16914861E-06
TETRALIN	1.91848923E-10	2.53643462E-08
FLUORENE	3.09912235E-09	5.15167108E-07

TOTAL KG-MOLE FED/S = 1.71938695E-08
TOTAL KGS FED/S = 2.46260713E-06
PUMP RATE/ M3/S = 2.8405318E-09
TOTAL KG-ATOMS CARBON= 6.52444603E-04
TOTAL KG-ATOMS HYDROGEN= 1.02075592E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.760956
WHSV (1/S) LIQ FEED BASIS= 3.49580863E-04
VHSV (1/S) = 2.18500698E-04
TOTAL WHSV (1/S) = 5.53438305E-04
MOLAR GAS DENSITY =.262607357 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.64336351
SUPERFICIAL GAS VELOCITY/ M/S = .0142841564

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.1134058E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.21683029E-07
H2 FEEDRATE KG-MOLE/S = 7.18032427E-07
FRACTION OF GAS THAT IS HYDROCARBONS =4.66378815E-03
KG-MOLE/S FREE H2 IN GAS= 7.18317253E-07
H BALANCE CLOSURE = 98.7482141 C BALANCE CLOSURE=93.3828467

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	1.24428903E-03	1	.335166251
	2	2.36213224E-04	2	.0636272592
	3	5.75616739E-05	3	.0155050233
	4	7.72266912E-04	4	.208020644
	5	0	5	0
	6	3.39255978E-04	6	.0913832331
	7	1.85270461E-03	7	0
	8	7.30562785E-04	8	0
	9	3.83734185E-05	9	0
	10	3.67954192E-04	10	.0991134891
	11	3.71960453E-04	11	.10019263
	12	1.83598919E-04	12	.0494548774
	13	4.33348633E-04	13	0
	14	1.39352843E-04	14	.0375365921
	H2	.255839915		

KG-MOLE FLUORENE/S IN PRODUCT = 1.21670538E-09
FLUORENE CONVERSION = 60.7403245 %
T-DECALIN CONVERSION= 4.48613793 %
C-DECALIN CONVERSION= 75.7450175 %

RUN NUMBER =97 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN97TP
PUMP TEMP/ DEG K =385.372222
INITIAL TIME OF M. B./S =8502 FINAL TIME=12262.2
INITIAL PUMP VOL/M3= 6.922E-05 FINAL VOL/M3= 7.991E-05
WT % OF TRANS-DECALIN =30.575
CIS-DECALIN = 47.477
TETRALIN = 1.03
FLUORENE = 20.92
BAROMETRIC PRESSURE/ BARS =1.0117368
P CORRECTION/ BARS = 4.16478E-03
H20 VAPOR PRESS/ BARS = .03778776
WTM SEC/REV AVERAGE=78.3 WTM TEMP/K=300.372223
KGMS OF CATALYST =7.01E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=688.15
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.927778
KGS/SEC IN COND A=1.98060288E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =19803
GC AREA COUNTS, GAS 4 =110180 GAS 5 =100160
GC AREA COUNTS, GAS 6 =40425 GAS 7 =12580

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.121	27	1.754	1	0	27	0
2	.11	28	0	2	0	28	0
3	.355	29	29.881	3	0	29	0
4	.623	30	13.061	4	0	30	0
5	.208	31	2.415	5	0	31	0
6	4.023	32	3.953	6	0	32	0
7	2.168	33	.592	7	0	33	0
8	0	34	3.678	8	0	34	0
9	1.236	35	.058	9	0	35	0
10	.973	36	.187	10	0	36	0
11	.26	37	.353	11	0	37	0
12	0	38	.525	12	0	38	0
13	0	39	2.222	13	0	39	0
14	6.308	40	1.138	14	0	40	0
15	.083	41	.986	15	0	41	0
16	.079	42	.798	16	0	42	0
17	.057	43	.675	17	0	43	0
18	.074	44	1.094	18	0	44	0
19	.701	45	.61	19	0	45	0
20	3.677	46	1.148	20	0	46	0
21	1.162	47	.61	21	0	47	0
22	.978	48	3.876	22	0	48	0
23	1.316	49	.906	23	0	49	0
24	1.535	50	1.697	24	0	50	0
25	.597	51	0	25	0	51	0
26	1.14	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 97 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.45375455E-09	7.53981567E-07
C-DECALIN	8.46861505E-09	1.17078603E-06
TETRALIN	1.92117613E-10	2.53998696E-08
FLUORENE	3.10346276E-09	5.15888614E-07

TOTAL KG-MOLE FED/S = 1.721795E-08
TOTAL KGS FED/S = 2.46605608E-06
PUMP RATE/ M3/S = 2.84295663E-09
TOTAL KG-ATOMS CARBON= 6.5335837E-04
TOTAL KG-ATOMS HYDROGEN= 1.02218551E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 40.7726853
WHSV (1/S) LIQ FEED BASIS= 3.51788353E-04
VHSV (1/S) = 2.18687222E-04
TOTAL WHSV (1/S) = 5.52078349E-04
MOLAR GAS DENSITY =.258686263 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.67569698
SUPERFICIAL GAS VELOCITY/ M/S = .0141853783

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.98046029E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.00391375E-07
H2 FEEDRATE KG-MOLE/S = 7.02022054E-07
FRACTION OF GAS THAT IS HYDROCARBONS =9.99058138E-03
KG-MOLE/S FREE H2 IN GAS= 6.93394058E-07
H BALANCE CLOSURE = 98.6325652 C BALANCE CLOSURE=94.0868991

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	2.66000463E-03	1	.457502122
2	4.6068255E-04	2	.0792341644
3	7.98092557E-05	3	.0137266317
4	1.27887414E-03	4	.219957374
5	0	5	0
6	1.89738361E-04	6	.0326336661
7	1.54610635E-03	7	0
8	6.75803855E-04	8	0
9	3.20307256E-05	9	0
10	3.99489684E-04	10	.0687094211
11	4.85308115E-04	11	.0834695887
12	1.92937426E-04	12	.0331838828
13	1.66795273E-04	13	0
14	6.73466417E-05	14	.0115831496
H2	.250451336		

KG-MOLE FLUORENE/S IN PRODUCT = 4.61785723E-10
FLUORENE CONVERSION = 85.1203073 %
T-DECALIN CONVERSION= 21.5124925 %
C-DECALIN CONVERSION= 77.9064738 %

RUN NUMBER =98 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN98TP
PUMP TEMP/ DEG K =392.038889
INITIAL TIME OF M. B./S =7582.8 FINAL TIME=11231.4
INITIAL PUMP VOL/M3= 1.0403E-04 FINAL VOL/M3= 1.1439E-04
WT % OF TRANS-DECALIN =30.575
CIS-DECALIN = 47.477
TETRALIN = 1.03
FLUORENE = 20.918
BAROMETRIC PRESSURE/ BARS =1.0334072
P CORRECTION/ BARS = 3.41986E-03
H20 VAPOR PRESS/ BARS = .0348758
WTM SEC/REV AVERAGE=77.1 WTM TEMP/K=298.427778
KGMS OF CATALYST =7.0014E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=683.538889
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.538889
KGS/SEC IN COND A=1.93843284E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =9818
GC AREA COUNTS, GAS 4 =66149 GAS 5 =99317
GC AREA COUNTS, GAS 6 =23938 GAS 7 =12747

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.122	27	3.006	1	0	27	0
2	.065	28	2.958	2	0	28	0
3	.196	29	30.539	3	0	29	0
4	.284	30	5.829	4	0	30	0
5	.091	31	3.484	5	0	31	0
6	2.576	32	6.31	6	0	32	0
7	.491	33	0	7	0	33	0
8	0	34	4.763	8	0	34	0
9	.927	35	.139	9	0	35	0
10	.823	36	.277	10	0	36	0
11	.201	37	.371	11	0	37	0
12	.028	38	.511	12	0	38	0
13	0	39	1.916	13	0	39	0
14	1.862	40	.911	14	0	40	0
15	.11	41	.937	15	0	41	0
16	.084	42	.699	16	0	42	0
17	.093	43	.428	17	0	43	0
18	.166	44	.819	18	0	44	0
19	.424	45	.346	19	0	45	0
20	1.479	46	1.158	20	0	46	0
21	.887	47	.716	21	0	47	0
22	1.599	48	6.898	22	0	48	0
23	3.514	49	1.593	23	0	49	0
24	1.904	50	3.513	24	0	50	0
25	1.435	51	0	25	0	51	0
26	2.524	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 98 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.41117503E-09	7.48094948E-07
C-DECALIN	8.40249736E-09	1.16164526E-06
TETRALIN	1.90617678E-10	2.52015633E-08
FLUORENE	3.07893847E-09	5.11811942E-07

TOTAL KG-MOLE FED/S = 1.70832285E-08
TOTAL KGS FED/S = 2.44675371E-06
PUMP RATE/ M3/S = 2.83946798E-09
TOTAL KG-ATOMS CARBON= 6.48243577E-04
TOTAL KG-ATOMS HYDROGEN= 1.01419433E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 43.1026148
WHSV (1/S) LIQ FEED BASIS= 3.49463556E-04
VHSV (1/S) = 2.18418866E-04
TOTAL WHSV (1/S) = 5.59800326E-04
MOLAR GAS DENSITY =.260430876 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.49370966
SUPERFICIAL GAS VELOCITY/ M/S = .0147598612

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 1.93829328E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.44097678E-07
H2 FEEDRATE KG-MOLE/S = 7.3633182E-07
FRACTION OF GAS THAT IS HYDROCARBONS =7.27896293E-03
KG-MOLE/S FREE H2 IN GAS= 7.38681419E-07
H BALANCE CLOSURE = 98.7536583 C BALANCE CLOSURE=90.8021426

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	1.92751131E-03	1	.396736815
2	2.96549328E-04	2	.0610383115
3	6.77987393E-05	3	.0139549147
4	8.48438533E-04	4	.174632854
5	0	5	0
6	3.82819926E-04	6	.0787952619
7	1.46963391E-03	7	0
8	2.80510038E-04	8	0
9	0	9	0
10	5.51913814E-04	10	.113599608
11	4.48547858E-04	11	.0923239453
12	2.05168634E-04	12	.042229558
13	2.76078938E-04	13	0
14	1.29664881E-04	14	.0266887317
H2	.25354624		

KG-MOLE FLUORENE/S IN PRODUCT = 8.04328164E-10
FLUORENE CONVERSION = 73.8764457 %
T-DECALIN CONVERSION= 20.8742971 %
C-DECALIN CONVERSION= 90.2738711 %

RUN NUMBER =99 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN99TP
PUMP TEMP/ DEG K =393.705556
INITIAL TIME OF M. B./S =8520 FINAL TIME=12247.2
INITIAL PUMP VOL/M3= 1.3858E-04 FINAL VOL/M3= 1.4917E-04
WT % OF TRANS-DECALIN =30.575
CIS-DECALIN = 47.477
TETRALIN = 1.03
FLUORENE = 20.92
BAROMETRIC PRESSURE/ BARS =1.0205404
P CORRECTION/ BARS = 4.19864E-03
H20 VAPOR PRESS/ BARS = .0348758
WTM SEC/REV AVERAGE=78 WTM TEMP/K=298.983334
KGMS OF CATALYST =7.0017E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=694.538889
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.538889
KGS/SEC IN COND A=2.01452226E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =295.927778
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =12821
GC AREA COUNTS, GAS 4 =62329 GAS 5 =68259
GC AREA COUNTS, GAS 6 =21497 GAS 7 =10592

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.081	27	1.993	1	0	27	0
2	.045	28	2.384	2	0	28	0
3	.076	29	32.932	3	0	29	0
4	.14	30	17.253	4	0	30	0
5	.045	31	2.399	5	0	31	0
6	1.258	32	3.973	6	0	32	0
7	.568	33	.635	7	0	33	0
8	0	34	4.182	8	0	34	0
9	.503	35	.026	9	0	35	0
10	.482	36	.071	10	0	36	0
11	.136	37	.14	11	0	37	0
12	0	38	.221	12	0	38	0
13	.019	39	1.69	13	0	39	0
14	2.14	40	.69	14	0	40	0
15	.059	41	.639	15	0	41	0
16	.045	42	.474	16	0	42	0
17	.053	43	.323	17	0	43	0
18	.079	44	.577	18	0	44	0
19	.381	45	.227	19	0	45	0
20	1.834	46	.938	20	0	46	0
21	.645	47	.717	21	0	47	0
22	.997	48	7.123	22	0	48	0
23	1.94	49	1.283	23	0	49	0
24	1.366	50	3.725	24	0	50	0
25	.891	51	0	25	0	51	0
26	1.608	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 99 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.40547992E-09	7.47307599E-07
C-DECALIN	8.39365398E-09	1.16042266E-06
TETRALIN	1.90417059E-10	2.51750393E-08
FLUORENE	3.07599204E-09	5.11322158E-07

TOTAL KG-MOLE FED/S = 1.7065543E-08
TOTAL KGS FED/S = 2.44422746E-06
PUMP RATE/ M3/S = 2.84129766E-09
TOTAL KG-ATOMS CARBON= 6.47575081E-04
TOTAL KG-ATOMS HYDROGEN= 1.0131375E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.9864806
WHSV (1/S) LIQ FEED BASIS= 3.49087779E-04
VHSV (1/S) = 2.1855961E-04
TOTAL WHSV (1/S) = 5.53757033E-04
MOLAR GAS DENSITY =.256307301 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.5420907
SUPERFICIAL GAS VELOCITY/ M/S = .0146026433

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.01437723E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.18417636E-07
H2 FEEDRATE KG-MOLE/S = 7.16522089E-07
FRACTION OF GAS THAT IS HYDROCARBONS =6.14809266E-03
KG-MOLE/S FREE H2 IN GAS= 7.14000737E-07
H BALANCE CLOSURE = 98.3863223 C BALANCE CLOSURE=91.5127282
PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	1.58143016E-03	1	.407239873
	2	1.60016817E-04	2	.0412065167
	3	4.15842646E-05	3	.0107085163
	4	7.76552701E-04	4	.199972931
	5	0	5	0
	6	2.45647483E-04	6	.0632575832
	7	1.67696163E-03	7	0
	8	8.7855639E-04	8	0
	9	3.38126789E-05	9	0
	10	3.61350788E-04	10	.0930527652
	11	3.99275157E-04	11	.102818808
	12	1.71945743E-04	12	.0442783781
	13	3.01664148E-04	13	0
	14	1.45485986E-04	14	.0374646293
	H2	.249533017		

KG-MOLE FLUORENE/S IN PRODUCT = 8.63166034E-10
FLUORENE CONVERSION = 71.9386129 %
T-DECALIN CONVERSION= 11.2313712 %
C-DECALIN CONVERSION= 70.0505243 %

RUN NUMBER =100 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN100FL
PUMP TEMP/ DEG K =387.594445
INITIAL TIME OF M. B./S =11073 FINAL TIME=14786.4
INITIAL PUMP VOL/M3= 9.41E-05 FINAL VOL/M3= 1.0464E-04
WT % OF TRANS-DECALIN =39
CIS-DECALIN = 59.59
TETRALIN = 1.27
FLUORENE = .14
BAROMETRIC PRESSURE/ BARS =1.0198632
P CORRECTION/ BARS = 4.36794E-03
H20 VAPOR PRESS/ BARS = .03778776
WTM SEC/REV AVERAGE=78 WTM TEMP/K=300.372223
KGMS OF CATALYST =7E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.65
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.927778
KGS/SEC IN COND A=1.8691773E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =295.372223
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =8049
GC AREA COUNTS, GAS 4 =53832 GAS 5 =125420
GC AREA COUNTS, GAS 6 =20746 GAS 7 =11283

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.507	27	3.36	1	0	27	0
2	.241	28	5.288	2	0	28	0
3	1.378	29	20.005	3	0	29	0
4	1.528	30	2.193	4	0	30	0
5	.55	31	3.359	5	0	31	0
6	12.045	32	6.298	6	0	32	0
7	.655	33	0	7	0	33	0
8	.694	34	3.108	8	0	34	0
9	2.742	35	.144	9	0	35	0
10	2.2	36	.267	10	0	36	0
11	.461	37	.805	11	0	37	0
12	.097	38	.81	12	0	38	0
13	.023	39	1.523	13	0	39	0
14	2.944	40	.772	14	0	40	0
15	.327	41	.331	15	0	41	0
16	.196	42	.472	16	0	42	0
17	.158	43	.662	17	0	43	0
18	.238	44	.207	18	0	44	0
19	.466	45	.093	19	0	45	0
20	1.902	46	.183	20	0	46	0
21	1.218	47	.198	21	0	47	0
22	4.927	48	.394	22	0	48	0
23	5.574	49	0	23	0	49	0
24	3.246	50	0	24	0	50	0
25	1.985	51	0	25	0	51	0
26	3.228	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 100 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	6.5803883E-09	9.09738683E-07
C-DECALIN	1.00544959E-08	1.39003405E-06
TETRALIN	2.24074002E-10	2.96248238E-08
FLUORENE	1.96458437E-11	3.26572861E-09

TOTAL KG-MOLE FED/S = 1.6878604E-08
TOTAL KGS FED/S = 2.33266329E-06
PUMP RATE/ M3/S = 2.83839186E-09
TOTAL KG-ATOMS CARBON= 6.07837057E-04
TOTAL KG-ATOMS HYDROGEN= 1.08831903E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.0935164
WHSV (1/S) LIQ FEED BASIS= 3.33234947E-04
VHSV (1/S) = 2.18336089E-04
TOTAL WHSV (1/S) = 5.3622755E-04
MOLAR GAS DENSITY =.269451265 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.81591259
SUPERFICIAL GAS VELOCITY/ M/S = .0137723701

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.86904273E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.15012801E-07
H2 FEEDRATE KG-MOLE/S = 7.10479794E-07
FRACTION OF GAS THAT IS HYDROCARBONS =7.41901593E-03
KG-MOLE/S FREE H2 IN GAS= 7.0970811E-07
H BALANCE CLOSURE = 97.8832295 C BALANCE CLOSURE=92.8675076

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	2.34096575E-03	1	.343872724
2	1.2443731E-03	2	.182790358
3	2.40872474E-04	3	.0353826081
4	1.46673673E-03	4	.215454137
5	0	5	0
6	5.43956898E-04	6	.0799037492
7	9.96598383E-04	7	0
8	1.092497E-04	8	0
9	0	9	0
10	5.98500997E-04	10	.0879159244
11	3.22543421E-04	11	.0473795419
12	4.97023686E-05	12	7.3009564E-03
13	1.63242629E-05	13	0
14	0	14	0
H2	.261521441		

KG-MOLE FLUORENE/S IN PRODUCT = 4.43002368E-11

T-DECALIN CONVERSION= 58.900066 %
C-DECALIN CONVERSION= 97.0512876 %

RUN NUMBER =101 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN101SV
PUMP TEMP/ DEG K =388.705556
INITIAL TIME OF M. B./S =15642 FINAL TIME=19384.8
INITIAL PUMP VOL/M3= 6.915E-05 FINAL VOL/M3= 7.979E-05
WT % OF TRANS-DECALIN =28.252
CIS-DECALIN = 50.621
TETRALIN = 1.239
FLUORENE = 19.888
BAROMETRIC PRESSURE/ BARS =1.0229106
P CORRECTION/ BARS = 4.46952E-03
H20 VAPOR PRESS/ BARS = .0352144
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.261111
KGMS OF CATALYST =0 VOLUME/M3=0
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.816667
KGS/SEC IN COND A=2.65043424E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =0 GAS 5 =0
GC AREA COUNTS, GAS 6 =0 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	0	27	0	1	0	27	0
2	0	28	0	2	0	28	0
3	0	29	30.947	3	0	29	0
4	0	30	48.612	4	0	30	0
5	0	31	0	5	0	31	0
6	0	32	0	6	0	32	0
7	0	33	1.095	7	0	33	0
8	0	34	.062	8	0	34	0
9	0	35	0	9	0	35	0
10	0	36	.111	10	0	36	0
11	0	37	0	11	0	37	0
12	0	38	.063	12	0	38	0
13	0	39	.094	13	0	39	0
14	0	40	.036	14	0	40	0
15	0	41	0	15	0	41	0
16	0	42	.11	16	0	42	0
17	0	43	0	17	0	43	0
18	0	44	0	18	0	44	0
19	0	45	0	19	0	45	0
20	.062	46	0	20	0	46	0
21	0	47	0	21	0	47	0
22	0	48	17.809	22	0	48	0
23	0	49	.971	23	0	49	0
24	0	50	0	24	0	50	0
25	.029	51	0	25	0	51	0
26	0	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 101 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.01371813E-09	6.93146532E-07
C-DECALIN	8.98341447E-09	1.24195705E-06
TETRALIN	2.29923233E-10	3.03981507E-08
FLUORENE	2.93533426E-09	4.87940614E-07

TOTAL KG-MOLE FED/S = 1.71623901E-08
TOTAL KGS FED/S = 2.45344235E-06
PUMP RATE/ M3/S = 2.84281424E-09
TOTAL KG-ATOMS CARBON= 6.49542457E-04
TOTAL KG-ATOMS HYDROGEN= 1.02261073E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.7856508
WHSV (1/S) LIQ FEED BASIS= 0
VHSV (1/S) = 0
TOTAL WHSV (1/S) = 0
MOLAR GAS DENSITY =.26933805 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =0
SUPERFICIAL GAS VELOCITY/ M/S = 0

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.65024342E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.16043099E-07
H2 FEEDRATE KG-MOLE/S = 7.17141638E-07
FRACTION OF GAS THAT IS HYDROCARBONS =0
KG-MOLE/S FREE H2 IN GAS= 7.16043099E-07
H BALANCE CLOSURE = 101.302384 C BALANCE CLOSURE=107.939509

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	0	1	0
	2	0	2	0
	3	0	3	0
	4	5.67433005E-06	4	.059546089
	5	0	5	0
	6	2.0382506E-06	6	.0213892831
	7	2.17509453E-03	7	0
	8	3.41667028E-03	8	0
	9	8.04775107E-05	9	0
	10	1.1563702E-05	10	.121348815
	11	1.35827951E-05	11	.14253706
	12	6.24339993E-05	12	.655178752
	13	1.04100988E-03	13	0
	14	0	14	0
	H2	.262529505		

KG-MOLE FLUORENE/S IN PRODUCT = 2.83933015E-09

RUN NUMBER =101.1 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN101SVEXT
PUMP TEMP/ DEG K =388.705556
INITIAL TIME OF M. B./S =15642 FINAL TIME=19384.8
INITIAL PUMP VOL/M3= 6.915E-05 FINAL VOL/M3= 7.979E-05
WT % OF TRANS-DECALIN =28.252
CIS-DECALIN = 50.621
TETRALIN = 1.239
FLUORENE = 19.888
BAROMETRIC PRESSURE/ BARS =1.0229106
P CORRECTION/ BARS = 4.46952E-03
H20 VAPOR PRESS/ BARS = .0352144
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.261111
KGMS OF CATALYST =0 VOLUME/M3=0
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=633.15
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.816667
KGS/SEC IN COND A=2.65043424E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =0 GAS 5 =0
GC AREA COUNTS, GAS 6 =0 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	0	27	0	1	0	27	0
2	0	28	0	2	0	28	0
3	0	29	30.947	3	0	29	0
4	0	30	48.612	4	0	30	0
5	0	31	0	5	0	31	0
6	0	32	0	6	0	32	0
7	0	33	1.095	7	0	33	0
8	0	34	.062	8	0	34	0
9	0	35	0	9	0	35	0
10	0	36	.111	10	0	36	0
11	0	37	0	11	0	37	0
12	0	38	.063	12	0	38	0
13	0	39	.094	13	0	39	0
14	0	40	.036	14	0	40	0
15	0	41	0	15	0	41	0
16	0	42	.11	16	0	42	0
17	0	43	0	17	0	43	0
18	0	44	0	18	0	44	0
19	0	45	0	19	0	45	0
20	.062	46	0	20	0	46	0
21	0	47	0	21	0	47	0
22	0	48	17.809	22	0	48	0
23	0	49	.971	23	0	49	0
24	0	50	0	24	0	50	0
25	.029	51	0	25	0	51	0
26	0	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 101.1 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.01371813E-09	6.93146532E-07
C-DECALIN	8.98341447E-09	1.24195705E-06
TETRALIN	2.29923233E-10	3.03981507E-08
FLUORENE	2.93533426E-09	4.87940614E-07

TOTAL KG-MOLE FED/S = 1.71623901E-08
TOTAL KGS FED/S = 2.45344235E-06
PUMP RATE/ M3/S = 2.84281424E-09
TOTAL KG-ATOMS CARBON= 6.49542457E-04
TOTAL KG-ATOMS HYDROGEN= 1.02261073E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.7856508
WHSV (1/S) LIQ FEED BASIS= 0
WHSV (1/S) = 0
TOTAL WHSV (1/S) = 0
MOLAR GAS DENSITY =.281151122 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =0
SUPERFICIAL GAS VELOCITY/ M/S = 0

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.65024342E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.16043099E-07
H2 FEEDRATE KG-MOLE/S = 7.17141638E-07
FRACTION OF GAS THAT IS HYDROCARBONS =0
KG-MOLE/S FREE H2 IN GAS= 7.16043099E-07
H BALANCE CLOSURE = 101.302384 C BALANCE CLOSURE=107.939509

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	0	1	0
	2	0	2	0
	3	0	3	0
	4	5.92320417E-06	4	.059546089
	5	0	5	0
	6	2.12764756E-06	6	.0213892831
	7	2.27049341E-03	7	0
	8	3.56652424E-03	8	0
	9	8.40072261E-05	9	0
	10	1.20708819E-05	10	.121348815
	11	1.41785317E-05	11	.14253706
	12	6.51723326E-05	12	.655178752
	13	1.0866682E-03	13	0
	14	0	14	0
	H2	.274043957		

KG-MOLE FLUORENE/S IN PRODUCT = 2.83933015E-09

RUN NUMBER =102 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN102SV
PUMP TEMP/ DEG K =388.705556
INITIAL TIME OF M. B./S =8567.4 FINAL TIME=12274.2
INITIAL PUMP VOL/M3= 1.0212E-04 FINAL VOL/M3= 1.1264E-04
WT % OF TRANS-DECALIN =28.252
CIS-DECALIN = 50.621
TETRALIN = 1.239
FLUORENE = 19.888
BAROMETRIC PRESSURE/ BARS =1.0252808
P CORRECTION/ BARS = 4.30022E-03
H20 VAPOR PRESS/ BARS = .034208758
WTM SEC/REV AVERAGE=78 WTM TEMP/K=298.705556
KGMS OF CATALYST =1.0006E-03 VOLUME/M3=2.5E-06
REACTOR PRESS/BARS=15.0101392 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.261111
KGS/SEC IN COND A=2.41594326E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =295.372223
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =134
GC AREA COUNTS, GAS 4 =10824 GAS 5 =14508
GC AREA COUNTS, GAS 6 =4956 GAS 7 =2746

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.016	27	.613	1	0	27	0
2	.011	28	0	2	0	28	0
3	.014	29	35.191	3	0	29	0
4	.038	30	39.442	4	0	30	0
5	.016	31	.966	5	0	31	0
6	.664	32	.876	6	0	32	0
7	.061	33	0	7	0	33	0
8	.223	34	1.213	8	0	34	0
9	.258	35	.011	9	0	35	0
10	.238	36	.017	10	0	36	0
11	.066	37	.02	11	0	37	0
12	0	38	.069	12	0	38	0
13	0	39	.302	13	0	39	0
14	.488	40	.106	14	0	40	0
15	.031	41	.232	15	0	41	0
16	.024	42	.18	16	0	42	0
17	.022	43	.057	17	0	43	0
18	.076	44	.147	18	0	44	0
19	.073	45	.07	19	0	45	0
20	.213	46	.277	20	0	46	0
21	.092	47	.114	21	0	47	0
22	.419	48	12.22	22	0	48	0
23	.907	49	1.351	23	0	49	0
24	.345	50	1.094	24	0	50	0
25	.404	51	0	25	0	51	0
26	.735	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 102 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.00531591E-09	6.91984924E-07
C-DECALIN	8.96835963E-09	1.23987572E-06
TETRALIN	2.29537917E-10	3.0347208E-08
FLUORENE	2.93041509E-09	4.871229E-07

TOTAL KG-MOLE FED/S = 1.71336285E-08
TOTAL KGS FED/S = 2.44933075E-06
PUMP RATE/ M3/S = 2.83805011E-09
TOTAL KG-ATOMS CARBON= 6.48453923E-04
TOTAL KG-ATOMS HYDROGEN= 1.02089699E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.0847902
WHSV (1/S) LIQ FEED BASIS= 2.44784245E-03
VHSV (1/S) = 1.13521096E-03
TOTAL WHSV (1/S) = 3.88909649E-03
MOLAR GAS DENSITY =.273101507 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =.924898872
SUPERFICIAL GAS VELOCITY/ M/S = .0137908072

MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 2.41576932E-06 KGS/S,COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.26950282E-07
H2 FEEDRATE KG-MOLE/S = 7.21065162E-07
FRACTION OF GAS THAT IS HYDROCARBONS =1.11505768E-03
KG-MOLE/S FREE H2 IN GAS= 7.26139691E-07
H BALANCE CLOSURE = 100.985202 C BALANCE CLOSURE=100.146935
PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	3.08837317E-04	1	.255546669
	2	1.07089716E-04	2	.0886111188
	3	4.91621035E-05	3	.0406790601
	4	1.95986375E-04	4	.162168438
	5	0	5	0
	6	1.23367404E-04	6	.102080051
	7	2.2564565E-03	7	0
	8	2.52903178E-03	8	0
	9	0	9	0
	10	1.30599006E-04	10	.108063822
	11	1.25084236E-04	11	.10350064
	12	1.14607207E-04	12	.094831448
	13	6.51661853E-04	13	0
	14	5.38025112E-05	14	.0445187539
	H2	.266455821		

KG-MOLE FLUORENE/S IN PRODUCT = 1.77589491E-09
FLUORENE CONVERSION = 39.3978375 %
T-DECALIN CONVERSION= -22.8543216 %
C-DECALIN CONVERSION= 23.1513512 %

RUN NUMBER =103 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN103SV
PUMP TEMP/ DEG K =392.594445
INITIAL TIME OF M. B./S =8550 FINAL TIME=12247.8
INITIAL PUMP VOL/M3= 1.3548E-04 FINAL VOL/M3= 1.4598E-04
WT % OF TRANS-DECALIN =28.252
CIS-DECALIN = 50.621
TETRALIN = 1.239
FLUORENE = 19.888
BAROMETRIC PRESSURE/ BARS =1.0151228
P CORRECTION/ BARS = 4.33408E-03
H20 VAPOR PRESS/ BARS = .03778776
WTM SEC/REV AVERAGE=77.4 WTM TEMP/K=300.372223
KGMS OF CATALYST =3.0014E-03 VOLUME/M3=6.6E-06
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.927778
KGS/SEC IN COND A=2.2986561E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =295.372223
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =1818
GC AREA COUNTS, GAS 4 =34583 GAS 5 =61303
GC AREA COUNTS, GAS 6 =13743 GAS 7 =1978

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.048	27	1.67	1	0	27	0
2	.026	28	2.557	2	0	28	0
3	.114	29	35.428	3	0	29	0
4	.295	30	21.761	4	0	30	0
5	.099	31	1.796	5	0	31	0
6	2.9	32	2.855	6	0	32	0
7	.556	33	1.073	7	0	33	0
8	.211	34	2.287	8	0	34	0
9	.954	35	.039	9	0	35	0
10	.802	36	.097	10	0	36	0
11	.184	37	.092	11	0	37	0
12	.026	38	.195	12	0	38	0
13	.012	39	.689	13	0	39	0
14	1.467	40	.268	14	0	40	0
15	.093	41	.379	15	0	41	0
16	.057	42	.283	16	0	42	0
17	.042	43	.103	17	0	43	0
18	.098	44	.298	18	0	44	0
19	.198	45	.055	19	0	45	0
20	.633	46	.479	20	0	46	0
21	.314	47	.224	21	0	47	0
22	.945	48	7.464	22	0	48	0
23	2.482	49	1.431	23	0	49	0
24	.952	50	1.787	24	0	50	0
25	1.104	51	0	25	0	51	0
26	2.082	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 103 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	4.98852606E-09	6.89663727E-07
C-DECALIN	8.93827614E-09	1.23571668E-06
TETRALIN	2.28767954E-10	3.02454112E-08
FLUORENE	2.92058529E-09	4.85488893E-07

TOTAL KG-MOLE FED/S = 1.70761555E-08
TOTAL KGS FED/S = 2.44111471E-06
PUMP RATE/ M3/S = 2.83954892E-09
TOTAL KG-ATOMS CARBON= 6.46278747E-04
TOTAL KG-ATOMS HYDROGEN= 1.01747249E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.7272339
WHSV (1/S) LIQ FEED BASIS= 8.13318845E-04
VHSV (1/S) = 4.30231243E-04
TOTAL WHSV (1/S) = 1.28812063E-03
MOLAR GAS DENSITY =.26933805 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =2.43640928
SUPERFICIAL GAS VELOCITY/ M/S = .0138209412

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.29849061E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.14572755E-07
H2 FEEDRATE KG-MOLE/S = 7.12540731E-07
FRACTION OF GAS THAT IS HYDROCARBONS =3.86304055E-03
KG-MOLE/S FREE H2 IN GAS= 7.11812331E-07
H BALANCE CLOSURE = 100.330232 C BALANCE CLOSURE=99.8353475

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	1.07868622E-03	1	.314300843
	2	4.04058984E-04	2	.117732179
	3	1.00473507E-04	3	.0292753419
	4	7.46085524E-04	4	.217389733
	5	0	5	0
	6	3.21588028E-04	6	.093702308
	7	2.16765995E-03	7	0
	8	1.33144541E-03	8	0
	9	6.86507163E-05	9	0
	10	3.22043941E-04	10	.0938351488
	11	2.32909498E-04	11	.0678637125
	12	1.42311729E-04	12	.0414659014
	13	3.79814799E-04	13	0
	14	8.38607873E-05	14	.0244348316
	H2	.261958461		

KG-MOLE FLUORENE/S IN PRODUCT = 1.03206003E-09
FLUORENE CONVERSION = 64.6625615 %
T-DECALIN CONVERSION= -18.0733771 %
C-DECALIN CONVERSION= 59.5235258 %

RUN NUMBER =104 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN104SV
PUMP TEMP/ DEG K =388.705556
INITIAL TIME OF M. B./S =8988 FINAL TIME=12750.6
INITIAL PUMP VOL/M3= 1.7095E-04 FINAL VOL/M3= 1.8184E-04
WT % OF TRANS-DECALIN =28.252
CIS-DECALIN = 50.621
TETRALIN = 1.239
FLUORENE = 19.888
BAROMETRIC PRESSURE/ BARS =1.0300212
P CORRECTION/ BARS = 4.19864E-03
H20 VAPOR PRESS/ BARS = .0330135
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.261111
KGMS OF CATALYST =5.026E-04 VOLUME/M3=1E-06
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=298.705556
KGS/SEC IN COND A=2.25681942E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =294.261111
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =6678 GAS 5 =11010
GC AREA COUNTS, GAS 6 =2537 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	9E-03	27	.412	1	0	27	0
2	0	28	0	2	0	28	0
3	5E-03	29	34.59	3	0	29	0
4	0	30	39.098	4	0	30	0
5	0	31	.999	5	0	31	0
6	.321	32	.968	6	0	32	0
7	.027	33	0	7	0	33	0
8	.011	34	1.114	8	0	34	0
9	.119	35	.015	9	0	35	0
10	.153	36	.037	10	0	36	0
11	.028	37	.023	11	0	37	0
12	0	38	.062	12	0	38	0
13	.012	39	.242	13	0	39	0
14	.199	40	.083	14	0	40	0
15	.025	41	.216	15	0	41	0
16	.014	42	.211	16	0	42	0
17	9E-03	43	0	17	0	43	0
18	.068	44	.247	18	0	44	0
19	.037	45	.261	19	0	45	0
20	.1	46	0	20	0	46	0
21	.06	47	0	21	0	47	0
22	.478	48	14.818	22	0	48	0
23	.891	49	1.467	23	0	49	0
24	.26	50	1.121	24	0	50	0
25	.409	51	0	25	0	51	0
26	.781	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 104 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.10451797E-09	7.05699609E-07
C-DECALIN	9.14610661E-09	1.26444924E-06
TETRALIN	2.34087207E-10	3.09486697E-08
FLUORENE	2.98849398E-09	4.96777355E-07

TOTAL KG-MOLE FED/S = 1.74732058E-08
TOTAL KGS FED/S = 2.49787487E-06
PUMP RATE/ M3/S = 2.8942984E-09
TOTAL KG-ATOMS CARBON= 6.61305853E-04
TOTAL KG-ATOMS HYDROGEN= 1.04113049E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.4423548
WHSV (1/S) LIQ FEED BASIS= 4.96986648E-03
VHSV (1/S) = 2.89427525E-03
TOTAL WHSV (1/S) = 7.85138259E-03
MOLAR GAS DENSITY =.26933805 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =.36318602
SUPERFICIAL GAS VELOCITY/ M/S = .0140480099

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.25665694E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.21890446E-07
H2 FEEDRATE KG-MOLE/S = 7.24130793E-07
FRACTION OF GAS THAT IS HYDROCARBONS =6.88827008E-04
KG-MOLE/S FREE H2 IN GAS= 7.21393188E-07
H BALANCE CLOSURE = 98.2931643 C BALANCE CLOSURE=91.3647804

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	1.83358902E-04	1	.207220501
	2	5.0651066E-05	2	.0572425946
	3	1.64079731E-05	3	.0185432416
	4	1.40027709E-04	4	.158250359
	5	0	5	0
	6	1.02006933E-04	6	.11528171
	7	2.06099287E-03	7	0
	8	2.32959524E-03	8	0
	9	0	9	0
	10	1.30273554E-04	10	.147226837
	11	1.1719666E-04	11	.132448168
	12	9.36967853E-05	12	.105890113
	13	7.34296153E-04	13	0
	14	5.12296521E-05	14	.0578964756
	H2	.263328316		

KG-MOLE FLUORENE/S IN PRODUCT = 2.01161899E-09
FLUORENE CONVERSION = 32.6878686 %
T-DECALIN CONVERSION= -10.6104675 %
C-DECALIN CONVERSION= 30.221973 %

RUN NUMBER =105 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN105SV
PUMP TEMP/ DEG K =388.705556
INITIAL TIME OF M. B./S =8650.2 FINAL TIME=12366
INITIAL PUMP VOL/M3= 2.0567E-04 FINAL VOL/M3= 2.1622E-04
WT % OF TRANS-DECALIN =28.252
CIS-DECALIN = 50.621
TETRALIN = 1.239
FLUORENE = 19.888
BAROMETRIC PRESSURE/ BARS =1.0296826
P CORRECTION/ BARS = 4.50338E-03
H20 VAPOR PRESS/ BARS = .03480808
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.538889
KGMS OF CATALYST =2.0012E-03 VOLUME/M3=4.3E-06
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.538889
KGS/SEC IN COND A=2.21056572E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =295.372223
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =184
GC AREA COUNTS, GAS 4 =16156 GAS 5 =19978
GC AREA COUNTS, GAS 6 =6464 GAS 7 =3041

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.02	27	.862	1	0	27	0
2	.015	28	0	2	0	28	0
3	.034	29	35.109	3	0	29	0
4	.099	30	35.374	4	0	30	0
5	.036	31	0	5	0	31	0
6	1.262	32	1.453	6	0	32	0
7	.375	33	.81	7	0	33	0
8	0	34	1.665	8	0	34	0
9	.45	35	.011	9	0	35	0
10	.397	36	.034	10	0	36	0
11	.097	37	.033	11	0	37	0
12	0	38	.076	12	0	38	0
13	.015	39	.448	13	0	39	0
14	.812	40	.162	14	0	40	0
15	.051	41	.361	15	0	41	0
16	.031	42	.302	16	0	42	0
17	.025	43	.132	17	0	43	0
18	.085	44	.365	18	0	44	0
19	.124	45	.321	19	0	45	0
20	.394	46	.196	20	0	46	0
21	.15	47	.118	21	0	47	0
22	.534	48	10.703	22	0	48	0
23	1.146	49	1.653	23	0	49	0
24	.492	50	1.69	24	0	50	0
25	.516	51	0	25	0	51	0
26	.967	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 105 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.00743172E-09	6.92277435E-07
C-DECALIN	8.97215068E-09	1.24039983E-06
TETRALIN	2.29634946E-10	3.03600362E-08
FLUORENE	2.93165381E-09	4.87328813E-07

TOTAL KG-MOLE FED/S = 1.71408712E-08
TOTAL KGS FED/S = 2.45036612E-06
PUMP RATE/ M3/S = 2.8392498E-09
TOTAL KG-ATOMS CARBON= 6.46728033E-04
TOTAL KG-ATOMS HYDROGEN= 1.02132854E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.1030624
WHSV (1/S) LIQ FEED BASIS= 1.22443859E-03
VHSV (1/S) = 6.60285368E-04
TOTAL WHSV (1/S) = 1.94568324E-03
MOLAR GAS DENSITY =.26933805 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =1.56757606
SUPERFICIAL GAS VELOCITY/ M/S = .0139953499

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.21040657E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.27160175E-07
H2 FEEDRATE KG-MOLE/S = 7.21683168E-07
FRACTION OF GAS THAT IS HYDROCARBONS =1.55225446E-03
KG-MOLE/S FREE H2 IN GAS= 7.26031438E-07
H BALANCE CLOSURE = 99.550794 C BALANCE CLOSURE=92.4635935

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	4.30225909E-04	1	.275804077
	2	1.74106048E-04	2	.111613822
	3	3.78152083E-05	3	.0242421212
	4	2.92287801E-04	4	.187376365
	5	0	5	0
	6	1.46254695E-04	6	.0937592094
	7	2.03441207E-03	7	0
	8	2.04976766E-03	8	0
	9	4.90801994E-05	9	0
	10	9.64791952E-05	10	.0618497278
	11	1.80823142E-04	11	.115919936
	12	1.2679497E-04	12	.0812842017
	13	5.15800461E-04	13	0
	14	7.51098745E-05	14	.0481505395
	H2	.263129093		

KG-MOLE FLUORENE/S IN PRODUCT = 1.4232077E-09
FLUORENE CONVERSION = 51.45376 %
T-DECALIN CONVERSION= -12.1012478 %
C-DECALIN CONVERSION= 36.9631307 %

RUN NUMBER =106 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN106TP
PUMP TEMP/ DEG K =395.372222
INITIAL TIME OF M. B./S =15745.8 FINAL TIME=19533
INITIAL PUMP VOL/M3= 5.585E-05 FINAL VOL/M3= 6.641E-05
WT % OF TRANS-DECALIN =30.21
CIS-DECALIN = 48.09
TETRALIN = 1.05
FLUORENE = 20.65
BAROMETRIC PRESSURE/ BARS =1.024265
P CORRECTION/ BARS = 4.58803E-03
H20 VAPOR PRESS/ BARS = .03822794
WTM SEC/REV AVERAGE=79.2 WTM TEMP/K=299.816667
KGMS OF CATALYST =7.0001E-03 VOLUME/M3=1.33E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=622.594444
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=301.205556
KGS/SEC IN COND A=2.24465178E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =11782 GAS 5 =21739
GC AREA COUNTS, GAS 6 =4497 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.016	27	1.06	1	0	27	0
2	6E-03	28	3.433	2	0	28	0
3	.013	29	37.555	3	0	29	0
4	.039	30	18.424	4	0	30	0
5	.012	31	1.025	5	0	31	0
6	.877	32	1.558	6	0	32	0
7	.215	33	1.002	7	0	33	0
8	0	34	1.296	8	0	34	0
9	.354	35	.015	9	0	35	0
10	.367	36	.049	10	0	36	0
11	.06	37	.041	11	0	37	0
12	.012	38	.103	12	0	38	0
13	0	39	.318	13	0	39	0
14	.328	40	.154	14	0	40	0
15	.076	41	.456	15	0	41	0
16	.038	42	.472	16	0	42	0
17	.043	43	0	17	0	43	0
18	.092	44	.607	18	0	44	0
19	.079	45	.393	19	0	45	0
20	.158	46	.736	20	0	46	0
21	.145	47	.139	21	0	47	0
22	1.444	48	12.933	22	0	48	0
23	4.819	49	2.111	23	0	49	0
24	0	50	1.818	24	0	50	0
25	1.61	51	0	25	0	51	0
26	3.5	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 106 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.22980478E-09	7.23020511E-07
C-DECALIN	8.32510135E-09	1.15094526E-06
TETRALIN	1.9007495E-10	2.51298092E-08
FLUORENE	2.97310702E-09	4.94219581E-07

TOTAL KG-MOLE FED/S = 1.67180881E-08
TOTAL KGS FED/S = 2.39331516E-06
PUMP RATE/ M3/S = 2.78836198E-09
TOTAL KG-ATOMS CARBON= 6.33955656E-04
TOTAL KG-ATOMS HYDROGEN= 9.93593059E-04

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.0917373
WHSV (1/S) LIQ FEED BASIS= 3.41894547E-04
VHSV (1/S) = 2.096496E-04
TOTAL WHSV (1/S) = 5.42945316E-04
MOLAR GAS DENSITY =.285916396 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =5.2785369
SUPERFICIAL GAS VELOCITY/ M/S = .0128552938

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.24449018E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.03113858E-07
H2 FEEDRATE KG-MOLE/S = 7.03693373E-07
FRACTION OF GAS THAT IS HYDROCARBONS =1.29007751E-03
KG-MOLE/S FREE H2 IN GAS= 7.02206786E-07
H BALANCE CLOSURE = 98.8357538 C BALANCE CLOSURE=96.0399265

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	3.70827615E-04	1	.153695688
2	1.41879113E-04	2	.0588041638
3	4.28079645E-05	3	.0177424746
4	7.10252069E-04	4	.294375812
5	0	5	0
6	4.8330003E-04	6	.200311755
7	2.42359896E-03	7	0
8	1.18898648E-03	8	0
9	6.76178796E-05	9	0
10	1.87000785E-04	10	.0775055932
11	1.76922317E-04	11	.073328404
12	2.09762964E-04	12	.0869397579
13	6.94141491E-04	13	0
14	8.99863708E-05	14	.0372963517
H2	.279129312		

KG-MOLE FLUORENE/S IN PRODUCT = 1.74625468E-09
FLUORENE CONVERSION = 41.2649911 %
T-DECALIN CONVERSION= -16.582901 %
C-DECALIN CONVERSION= 64.0708482 %

RUN NUMBER =107 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN107TP
PUMP TEMP/ DEG K =395.927778
INITIAL TIME OF M. B./S =9373.8 FINAL TIME=13022.4
INITIAL PUMP VOL/M3= 9.442E-05 FINAL VOL/M3= 1.0478E-04
WT % OF TRANS-DECALIN =30.21
CIS-DECALIN = 48.09
TETRALIN = 1.05
FLUORENE = 20.65
BAROMETRIC PRESSURE/ BARS =1.0181702
P CORRECTION/ BARS = 4.19864E-03
H20 VAPOR PRESS/ BARS = .03650108
WTM SEC/REV AVERAGE=78.3 WTM TEMP/K=300.372223
KGMS OF CATALYST =6.9993E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=611.205556
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.372223
KGS/SEC IN COND A=1.97690814E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =296.483334
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =6788 GAS 5 =14853
GC AREA COUNTS, GAS 6 =2829 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.067	27	0	1	0	27	0
2	.024	28	5.268	2	0	28	0
3	.018	29	38.132	3	0	29	0
4	.042	30	9.948	4	0	30	0
5	7E-03	31	.92	5	0	31	0
6	.964	32	1.448	6	0	32	0
7	.232	33	1.39	7	0	33	0
8	0	34	.957	8	0	34	0
9	.342	35	.046	9	0	35	0
10	.399	36	.081	10	0	36	0
11	.06	37	.07	11	0	37	0
12	.01	38	.251	12	0	38	0
13	0	39	.45	13	0	39	0
14	.244	40	.282	14	0	40	0
15	.085	41	.774	15	0	41	0
16	.04	42	.928	16	0	42	0
17	.067	43	0	17	0	43	0
18	.111	44	1.263	18	0	44	0
19	.102	45	.185	19	0	45	0
20	.137	46	.357	20	0	46	0
21	.185	47	.145	21	0	47	0
22	2.012	48	12.401	22	0	48	0
23	6.94	49	2.294	23	0	49	0
24	0	50	1.798	24	0	50	0
25	2.291	51	0	25	0	51	0
26	6.236	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 107 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.32264615E-09	7.3585583E-07
C-DECALIN	8.47289153E-09	1.17137725E-06
TETRALIN	1.93449229E-10	2.55759226E-08
FLUORENE	3.02588669E-09	5.02993144E-07

TOTAL KG-MOLE FED/S = 1.70148736E-08
TOTAL KGS FED/S = 2.43580215E-06
PUMP RATE/ M3/S = 2.83946798E-09
TOTAL KG-ATOMS CARBON= 6.45209864E-04
TOTAL KG-ATOMS HYDROGEN= 1.01123168E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.5863255
WHSV (1/S) LIQ FEED BASIS= 3.48003753E-04
VHSV (1/S) = 2.18418867E-04
TOTAL WHSV (1/S) = 5.50189803E-04
MOLAR GAS DENSITY =.291242417 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =5.22519565
SUPERFICIAL GAS VELOCITY/ M/S = .0126935975

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 1.97676581E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.2887998E-07
H2 FEEDRATE KG-MOLE/S = 7.07586071E-07
FRACTION OF GAS THAT IS HYDROCARBONS =8.25451456E-04
KG-MOLE/S FREE H2 IN GAS= 7.28278325E-07
H BALANCE CLOSURE = 99.0323868 C BALANCE CLOSURE=82.8863979

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	2.54224072E-04	1	.101282184
	2	1.31552331E-04	2	.0524100937
	3	4.19683322E-05	3	.0167200703
	4	9.45532956E-04	4	.376697779
	5	0	5	0
	6	5.1720619E-04	6	.206053551
	7	2.13650812E-03	7	0
	8	5.57379176E-04	8	0
	9	8.14386561E-05	9	0
	10	1.62473212E-04	10	.0647288894
	11	1.69495479E-04	11	.0675265414
	12	2.10337503E-04	12	.0837978938
	13	5.7786635E-04	13	0
	14	7.7267083E-05	14	.0307829974
	H2	.285379167		

KG-MOLE FLUORENE/S IN PRODUCT = 1.47469607E-09
FLUORENE CONVERSION = 51.264002 %
T-DECALIN CONVERSION= -2.43587258 %
C-DECALIN CONVERSION= 83.2121836 %

RUN NUMBER =108 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN108TP
PUMP TEMP/ DEG K =394.816667
INITIAL TIME OF M. B./S =9125.4 FINAL TIME=12894
INITIAL PUMP VOL/M3= 1.298E-04 FINAL VOL/M3= 1.405E-04
WT % OF TRANS-DECALIN =30.21
CIS-DECALIN = 48.09
TETRALIN = 1.05
FLUORENE = 20.65
BAROMETRIC PRESSURE/ BARS =1.0198632
P CORRECTION/ BARS = 4.7404E-03
H20 VAPOR PRESS/ BARS = .035227944
WTM SEC/REV AVERAGE=78.9 WTM TEMP/K=299.816667
KGMS OF CATALYST =7.0071E-03 VOLUME/M3=1.32E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=632.816667
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.538889
KGS/SEC IN COND A=2.36774496E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =296.483334
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =15646 GAS 5 =31180
GC AREA COUNTS, GAS 6 =5819 GAS 7 =4814

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.021	27	1.247	1	0	27	0
2	9E-03	28	3.687	2	0	28	0
3	.036	29	37.246	3	0	29	0
4	.095	30	15.183	4	0	30	0
5	.031	31	1.36	5	0	31	0
6	1.537	32	2.026	6	0	32	0
7	.274	33	1.076	7	0	33	0
8	0	34	1.528	8	0	34	0
9	.524	35	.045	9	0	35	0
10	.553	36	.108	10	0	36	0
11	.1	37	.114	11	0	37	0
12	.021	38	.266	12	0	38	0
13	0	39	.61	13	0	39	0
14	.479	40	.366	14	0	40	0
15	.1	41	.852	15	0	41	0
16	.05	42	.632	16	0	42	0
17	.051	43	0	17	0	43	0
18	.092	44	.177	18	0	44	0
19	.094	45	.138	19	0	45	0
20	.189	46	.497	20	0	46	0
21	.163	47	.213	21	0	47	0
22	1.587	48	11.817	22	0	48	0
23	5.26	49	2.145	23	0	49	0
24	0	50	2.006	24	0	50	0
25	1.734	51	0	25	0	51	0
26	3.664	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 108 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.32830094E-09	7.36637605E-07
C-DECALIN	8.48189315E-09	1.17262173E-06
TETRALIN	1.9365475E-10	2.56030945E-08
FLUORENE	3.0291014E-09	5.03527525E-07

TOTAL KG-MOLE FED/S = 1.70329502E-08
TOTAL KGS FED/S = 2.43838995E-06
PUMP RATE/ M3/S = 2.83927336E-09
TOTAL KG-ATOMS CARBON= 6.45895336E-04
TOTAL KG-ATOMS HYDROGEN= 1.01230601E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.4050668
WHSV (1/S) LIQ FEED BASIS= 3.47985678E-04
VHSV (1/S) = 2.15094746E-04
TOTAL WHSV (1/S) = 5.49280023E-04
MOLAR GAS DENSITY =.281299175 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =5.14088909
SUPERFICIAL GAS VELOCITY/ M/S = .0131002513

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.3675745E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.09388061E-07
H2 FEEDRATE KG-MOLE/S = 7.05250442E-07
FRACTION OF GAS THAT IS HYDROCARBONS =1.90851516E-03
KG-MOLE/S FREE H2 IN GAS= 7.08034183E-07
H BALANCE CLOSURE = 100.075378 C BALANCE CLOSURE=100.351942

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	5.46827827E-04	1	.182435574
	2	2.38948971E-04	2	.0797194118
	3	6.39526454E-05	3	.0213362178
	4	7.99893869E-04	4	.266864798
	5	0	5	0
	6	5.46352412E-04	6	.182276964
	7	2.4692928E-03	7	0
	8	1.00658521E-03	8	0
	9	7.45943711E-05	9	0
	10	2.68149004E-04	10	.0894612806
	11	1.9063992E-04	11	.0636022924
	12	2.40607147E-04	12	.0802726213
	13	6.51562261E-04	13	0
	14	1.02003188E-04	14	.0340308399
	H2	.274099765		

KG-MOLE FLUORENE/S IN PRODUCT = 1.6830673E-09
FLUORENE CONVERSION = 44.4367459 %
T-DECALIN CONVERSION= -19.7097177 %
C-DECALIN CONVERSION= 69.3448597 %

RUN NUMBER =109 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN109SV
PUMP TEMP/ DEG K =395.927778
INITIAL TIME OF M. B./S =8884.8 FINAL TIME=12636.6
INITIAL PUMP VOL/M3= 1.7792E-04 FINAL VOL/M3= 1.8858E-04
WT % OF TRANS-DECALIN =30.21
CIS-DECALIN = 48.09
TETRALIN = 1.05
FLUORENE = 20.65
BAROMETRIC PRESSURE/ BARS =1.0215562
P CORRECTION/ BARS = 4.94356E-03
H20 VAPOR PRESS/ BARS = .03778776
WTM SEC/REV AVERAGE=78.3 WTM TEMP/K=300.372223
KGMS OF CATALYST =1.0004E-03 VOLUME/M3=2.4E-06
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=633.705556
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.927778
KGS/SEC IN COND A=2.36177226E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =298.15
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =7838 GAS 5 =12788
GC AREA COUNTS, GAS 6 =2519 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	0	27	.548	1	0	27	0
2	.02	28	1.311	2	0	28	0
3	.01	29	34.625	3	0	29	0
4	0	30	35.426	4	0	30	0
5	0	31	.934	5	0	31	0
6	.102	32	.982	6	0	32	0
7	.028	33	0	7	0	33	0
8	0	34	.999	8	0	34	0
9	.054	35	.027	9	0	35	0
10	.051	36	.061	10	0	36	0
11	.011	37	.076	11	0	37	0
12	0	38	.201	12	0	38	0
13	0	39	.477	13	0	39	0
14	.078	40	.297	14	0	40	0
15	6E-03	41	.793	15	0	41	0
16	6E-03	42	.139	16	0	42	0
17	.048	43	0	17	0	43	0
18	.033	44	.111	18	0	44	0
19	.051	45	.133	19	0	45	0
20	.044	46	.302	20	0	46	0
21	.026	47	.147	21	0	47	0
22	.614	48	14.904	22	0	48	0
23	1.372	49	1.738	23	0	49	0
24	0	50	1.312	24	0	50	0
25	.606	51	0	25	0	51	0
26	1.299	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 109 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.32612827E-09	7.36337233E-07
C-DECALIN	8.47843458E-09	1.17214358E-06
TETRALIN	1.93575785E-10	2.55926546E-08
FLUORENE	3.02786625E-09	5.03322207E-07

TOTAL KG-MOLE FED/S = 1.70260049E-08
TOTAL KGS FED/S = 2.43739568E-06
PUMP RATE/ M3/S = 2.84132559E-09
TOTAL KG-ATOMS CARBON= 6.45631967E-04
TOTAL KG-ATOMS HYDROGEN= 1.01189324E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.6167222
WHSV (1/S) LIQ FEED BASIS= 2.43640162E-03
VHSV (1/S) = 1.18387619E-03
TOTAL WHSV (1/S) = 3.85295669E-03
MOLAR GAS DENSITY =.280904715 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =.929139553
SUPERFICIAL GAS VELOCITY/ M/S = .0131787501

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.36160223E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.08503376E-07
H2 FEEDRATE KG-MOLE/S = 7.08566515E-07
FRACTION OF GAS THAT IS HYDROCARBONS =7.89482838E-04
KG-MOLE/S FREE H2 IN GAS= 7.07944025E-07
H BALANCE CLOSURE = 99.5142089 C BALANCE CLOSURE=98.1826933

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	2.21089284E-04	1	.181900841
	2	2.03223189E-05	2	.0167201541
	3	9.15353288E-06	3	7.53105395E-03
	4	2.66837288E-04	4	.219539934
	5	0	5	0
	6	1.67146378E-04	6	.137519405
	7	2.29114938E-03	7	0
	8	2.34415186E-03	8	0
	9	0	9	0
	10	1.55411779E-04	10	.127864782
	11	1.35372528E-04	11	.111377522
	12	1.73518712E-04	12	.142762232
	13	8.20204601E-04	13	0
	14	6.65866745E-05	14	.0547840756
	H2	.27423377		

KG-MOLE FLUORENE/S IN PRODUCT = 2.11738673E-09
FLUORENE CONVERSION = 30.0700046 %
T-DECALIN CONVERSION= -11.0503087 %
C-DECALIN CONVERSION= 28.6246822 %

RUN NUMBER =110 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN110SV
PUMP TEMP/ DEG K =397.594445
INITIAL TIME OF M. B./S =10477.8 FINAL TIME=14155.2
INITIAL PUMP VOL/M3= 2.1978E-04 FINAL VOL/M3= 2.3022E-04
WT % OF TRANS-DECALIN =30.21
CIS-DECALIN = 48.09
TETRALIN = 1.05
FLUORENE = 20.65
BAROMETRIC PRESSURE/ BARS =1.019186
P CORRECTION/ BARS = 4.7404E-03
H20 VAPOR PRESS/ BARS = .031483028
WTM SEC/REV AVERAGE=77.1 WTM TEMP/K=297.038889
KGMS OF CATALYST =5.073E-04 VOLUME/M3=1.2E-06
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=632.761111
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=297.872223
KGS/SEC IN COND A=2.47647588E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =294.816667
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =3076 GAS 5 =5054
GC AREA COUNTS, GAS 6 =1433 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	0	27	.161	1	0	27	0
2	0	28	.504	2	0	28	0
3	0	29	31.878	3	0	29	0
4	0	30	43.675	4	0	30	0
5	0	31	0	5	0	31	0
6	.135	32	.133	6	0	32	0
7	.051	33	.929	7	0	33	0
8	0	34	.442	8	0	34	0
9	.081	35	0	9	0	35	0
10	.085	36	0	10	0	36	0
11	0	37	.068	11	0	37	0
12	0	38	.041	12	0	38	0
13	0	39	.106	13	0	39	0
14	.085	40	.025	14	0	40	0
15	0	41	.087	15	0	41	0
16	0	42	.081	16	0	42	0
17	0	43	0	17	0	43	0
18	.055	44	0	18	0	44	0
19	.02	45	.022	19	0	45	0
20	.041	46	0	20	0	46	0
21	.027	47	0	21	0	47	0
22	.162	48	17.994	22	0	48	0
23	.462	49	1.466	23	0	49	0
24	.101	50	.523	24	0	50	0
25	.169	51	0	25	0	51	0
26	.391	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 110 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.31267948E-09	7.34477938E-07
C-DECALIN	8.45702602E-09	1.16918385E-06
TETRALIN	1.93086995E-10	2.55280316E-08
FLUORENE	3.02022071E-09	5.02051288E-07

TOTAL KG-MOLE FED/S = 1.69830132E-08
TOTAL KGS FED/S = 2.4312411E-06
PUMP RATE/ M3/S = 2.838985E-09
TOTAL KG-ATOMS CARBON= 6.44001707E-04
TOTAL KG-ATOMS HYDROGEN= 1.00933815E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 43.0277589
WHSV (1/S) LIQ FEED BASIS= 4.7924732E-03
VHSV (1/S) = 2.36580191E-03
TOTAL WHSV (1/S) = 7.67335297E-03
MOLAR GAS DENSITY =.281323865 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =.451491906
SUPERFICIAL GAS VELOCITY/ M/S = .0135604845

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.47629759E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.33334764E-07
H2 FEEDRATE KG-MOLE/S = 7.30740998E-07
FRACTION OF GAS THAT IS HYDROCARBONS =3.25196342E-04
KG-MOLE/S FREE H2 IN GAS= 7.33096286E-07
H BALANCE CLOSURE = 100.656602 C BALANCE CLOSURE=102.370365

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	8.93663359E-05	1	.19220375
	2	2.70883102E-05	2	.0582599111
	3	8.03305104E-06	3	.0172770039
	4	1.1171566E-04	4	.240271333
	5	0	5	0
	6	5.31604811E-05	6	.114334371
	7	2.13970936E-03	7	0
	8	2.93154547E-03	8	0
	9	6.52049055E-05	9	0
	10	1.6253004E-05	10	.0349559852
	11	4.18515386E-05	11	.0900117765
	12	9.05629032E-05	12	.194777255
	13	1.00449359E-03	13	0
	14	2.6924973E-05	14	.0579086153
	H2	.274717956		

KG-MOLE FLUORENE/S IN PRODUCT = 2.48053292E-09
FLUORENE CONVERSION = 11.247118 %
T-DECALIN CONVERSION= -7.47690349 %
C-DECALIN CONVERSION= 7.49761269 %

RUN NUMBER =111 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN111SV
PUMP TEMP/ DEG K =388.15
INITIAL TIME OF M. B./S =9664.8 FINAL TIME=13368.6
INITIAL PUMP VOL/M3= 3.968E-05 FINAL VOL/M3= 5.019E-05
WT % OF TRANS-DECALIN =31.127
CIS-DECALIN = 48.187
TETRALIN = 1.088
FLUORENE = 19.599
BAROMETRIC PRESSURE/ BARS =1.0158
P CORRECTION/ BARS = 4.70654E-03
H20 VAPOR PRESS/ BARS = .035227944
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.538889
KGMS OF CATALYST =2.0011E-03 VOLUME/M3=4.2E-06
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=633.15
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.816667
KGS/SEC IN COND A=2.65260108E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =295.372223
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =11399 GAS 5 =19306
GC AREA COUNTS, GAS 6 =4907 GAS 7 =2918

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.012	27	.755	1	0	27	0
2	0	28	1.668	2	0	28	0
3	.015	29	34.675	3	0	29	0
4	.045	30	33.075	4	0	30	0
5	.011	31	0	5	0	31	0
6	.745	32	1.105	6	0	32	0
7	.196	33	.952	7	0	33	0
8	0	34	1.131	8	0	34	0
9	.232	35	.018	9	0	35	0
10	.257	36	.034	10	0	36	0
11	.05	37	.019	11	0	37	0
12	0	38	.073	12	0	38	0
13	0	39	.228	13	0	39	0
14	.287	40	.084	14	0	40	0
15	.046	41	.312	15	0	41	0
16	.026	42	.241	16	0	42	0
17	.03	43	0	17	0	43	0
18	.08	44	.225	18	0	44	0
19	.062	45	.123	19	0	45	0
20	.132	46	.362	20	0	46	0
21	.09	47	.129	21	0	47	0
22	.737	48	13.823	22	0	48	0
23	1.75	49	1.966	23	0	49	0
24	.425	50	1.463	24	0	50	0
25	.738	51	0	25	0	51	0
26	1.577	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 111 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.50828469E-09	7.61520358E-07
C-DECALIN	8.52725011E-09	1.17889233E-06
TETRALIN	2.01330162E-10	2.66178607E-08
FLUORENE	2.88448815E-09	4.79488466E-07

TOTAL KG-MOLE FED/S = 1.71213531E-08
TOTAL KGS FED/S = 2.44651901E-06
PUMP RATE/ M3/S = 2.83764892E-09
TOTAL KG-ATOMS CARBON= 6.47516004E-04
TOTAL KG-ATOMS HYDROGEN= 1.02203351E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.5336872
WHSV (1/S) LIQ FEED BASIS= 1.2225773E-03
VHSV (1/S) = 6.75625291E-04
TOTAL WHSV (1/S) = 1.93329365E-03
MOLAR GAS DENSITY =.281151122 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =1.62151686
SUPERFICIAL GAS VELOCITY/ M/S = .0132151394

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.65241011E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.18165559E-07
H2 FEEDRATE KG-MOLE/S = 7.11112925E-07
FRACTION OF GAS THAT IS HYDROCARBONS =1.28717094E-03
KG-MOLE/S FREE H2 IN GAS= 7.17241158E-07
H BALANCE CLOSURE = 102.365655 C BALANCE CLOSURE=110.543795

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	3.6334933E-04	1	.212435847
2	1.28166819E-04	2	.0749340225
3	3.33308857E-05	3	.0194872382
4	4.54904311E-04	4	.26596439
5	0	5	0
6	2.37314302E-04	6	.138748198
7	2.53742627E-03	7	0
8	2.42034244E-03	8	0
9	7.28475157E-05	9	0
10	9.45190099E-05	10	.0552614916
11	1.33990811E-04	11	.0783390778
12	1.82707236E-04	12	.106821627
13	8.41269232E-04	13	0
14	8.21128556E-05	14	.0480081084
H2	.273568841		

KG-MOLE FLUORENE/S IN PRODUCT = 2.20563466E-09
FLUORENE CONVERSION = 23.5346259 %
T-DECALIN CONVERSION= -20.7746051 %
C-DECALIN CONVERSION= 25.5839891 %

RUN NUMBER =112 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN112SV
PUMP TEMP/ DEG K =393.705556
INITIAL TIME OF M. B./S =11241.6 FINAL TIME=14951.4
INITIAL PUMP VOL/M3= 8.14E-05 FINAL VOL/M3= 9.194E-05
WT % OF TRANS-DECALIN =31.127
CIS-DECALIN = 48.187
TETRALIN = 1.088
FLUORENE = 19.599
BAROMETRIC PRESSURE/ BARS =1.017493
P CORRECTION/ BARS = 4.33408E-03
H20 VAPOR PRESS/ BARS = .036490922
WTM SEC/REV AVERAGE=78 WTM TEMP/K=299.261111
KGMS OF CATALYST =1E-03 VOLUME/M3=1.95E-06
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=633.705556
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.372223
KGS/SEC IN COND A=2.86442358E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =298.15
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =4519 GAS 5 =6514
GC AREA COUNTS, GAS 6 =2231 GAS 7 =1350

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	0	27	.137	1	0	27	0
2	0	28	.363	2	0	28	0
3	0	29	30.941	3	0	29	0
4	0	30	42.896	4	0	30	0
5	0	31	0	5	0	31	0
6	.118	32	.348	6	0	32	0
7	.042	33	.978	7	0	33	0
8	0	34	.627	8	0	34	0
9	.036	35	0	9	0	35	0
10	.059	36	0	10	0	36	0
11	0	37	.206	11	0	37	0
12	0	38	.197	12	0	38	0
13	0	39	.637	13	0	39	0
14	.093	40	.475	14	0	40	0
15	0	41	2.491	15	0	41	0
16	0	42	0	16	0	42	0
17	0	43	0	17	0	43	0
18	.022	44	.036	18	0	44	0
19	.049	45	0	19	0	45	0
20	.026	46	.249	20	0	46	0
21	.012	47	.076	21	0	47	0
22	.149	48	16.604	22	0	48	0
23	.337	49	.642	23	0	49	0
24	.095	50	.671	24	0	50	0
25	.115	51	0	25	0	51	0
26	.273	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 112 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.48460223E-09	7.58246257E-07
C-DECALIN	8.49058783E-09	1.17382377E-06
TETRALIN	2.00464558E-10	2.65034192E-08
FLUORENE	2.87208651E-09	4.77426941E-07

TOTAL KG-MOLE FED/S = 1.70477411E-08
TOTAL KGS FED/S = 2.43600039E-06
PUMP RATE/ M3/S = 2.84114624E-09
TOTAL KG-ATOMS CARBON= 6.44732057E-04
TOTAL KG-ATOMS HYDROGEN= 1.01763936E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.7860578
WHSV (1/S) LIQ FEED BASIS= 2.4359809E-03
VHSV (1/S) = 1.45698642E-03
TOTAL WHSV (1/S) = 3.86068529E-03
MOLAR GAS DENSITY =.280904715 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =.750979357
SUPERFICIAL GAS VELOCITY/ M/S = .0132480068

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.86421736E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.16267236E-07
H2 FEEDRATE KG-MOLE/S = 7.12357896E-07
FRACTION OF GAS THAT IS HYDROCARBONS =4.88000698E-04
KG-MOLE/S FREE H2 IN GAS= 7.15917697E-07
H BALANCE CLOSURE = 103.151262 C BALANCE CLOSURE=118.600021

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	1.33339521E-04	1	.167929036
2	2.14674886E-05	2	.0270363554
3	6.5652926E-06	3	8.26839071E-03
4	1.05853504E-04	4	.13331289
5	0	5	0
6	4.6549979E-05	6	.0586254776
7	2.44533599E-03	7	0
8	3.39016621E-03	8	0
9	8.08246596E-05	9	0
10	5.88756959E-05	10	.0741486003
11	1.41402337E-04	11	.178083421
12	2.39295234E-04	12	.301370649
13	1.09137162E-03	13	0
14	4.06739716E-05	14	.0512251791
H2	.273102993		

KG-MOLE FLUORENE/S IN PRODUCT = 2.86094357E-09
FLUORENE CONVERSION = .387973771 %
T-DECALIN CONVERSION= -16.8772656 %
C-DECALIN CONVERSION= -4.6694327 %

RUN NUMBER =113 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN113SV
PUMP TEMP/ DEG K =392.038889
INITIAL TIME OF M. B./S =8442 FINAL TIME=12143.4
INITIAL PUMP VOL/M3= 1.1506E-04 FINAL VOL/M3= 1.2558E-04
WT % OF TRANS-DECALIN =31.127
CIS-DECALIN = 48.187
TETRALIN = 1.088
FLUORENE = 19.599
BAROMETRIC PRESSURE/ BARS =1.0103824
P CORRECTION/ BARS = 4.50338E-03
H20 VAPOR PRESS/ BARS = .034208758
WTM SEC/REV AVERAGE=77.7 WTM TEMP/K=298.288889
KGMS OF CATALYST =4.13E-03 VOLUME/M3=8.1E-06
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=633.15
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.261111
KGS/SEC IN COND A=2.42149926E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =296.483334
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =14399 GAS 5 =29071
GC AREA COUNTS, GAS 6 =5730 GAS 7 =4622

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.021	27	1.389	1	0	27	0
2	0	28	4.014	2	0	28	0
3	.03	29	37.788	3	0	29	0
4	.075	30	13.421	4	0	30	0
5	.022	31	1.468	5	0	31	0
6	1.275	32	2.239	6	0	32	0
7	.173	33	1.119	7	0	33	0
8	0	34	1.602	8	0	34	0
9	.444	35	.046	9	0	35	0
10	.441	36	.103	10	0	36	0
11	.079	37	.087	11	0	37	0
12	.017	38	.219	12	0	38	0
13	0	39	.509	13	0	39	0
14	.373	40	.279	14	0	40	0
15	.083	41	.935	15	0	41	0
16	.044	42	.798	16	0	42	0
17	.054	43	0	17	0	43	0
18	.104	44	.785	18	0	44	0
19	.089	45	.099	19	0	45	0
20	.177	46	.374	20	0	46	0
21	.166	47	.151	21	0	47	0
22	1.73	48	11.451	22	0	48	0
23	5.823	49	2.254	23	0	49	0
24	0	50	1.557	24	0	50	0
25	1.931	51	0	25	0	51	0
26	4.162	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 113 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.49580829E-09	7.59795496E-07
C-DECALIN	8.50793569E-09	1.17622211E-06
TETRALIN	2.00874144E-10	2.65575706E-08
FLUORENE	2.87795472E-09	4.78402414E-07

TOTAL KG-MOLE FED/S = 1.70825728E-08
TOTAL KGS FED/S = 2.44097759E-06
PUMP RATE/ M3/S = 2.84219057E-09
TOTAL KG-ATOMS CARBON= 6.46049365E-04
TOTAL KG-ATOMS HYDROGEN= 1.01971859E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.7833098
WHSV (1/S) LIQ FEED BASIS= 5.91031008E-04
VHSV (1/S) = 3.50884917E-04
TOTAL WHSV (1/S) = 9.36677847E-04
MOLAR GAS DENSITY =.281151122 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =3.116023
SUPERFICIAL GAS VELOCITY/ M/S = .0132625884

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.42132493E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.16869354E-07
H2 FEEDRATE KG-MOLE/S = 7.13766433E-07
FRACTION OF GAS THAT IS HYDROCARBONS =1.78547655E-03
KG-MOLE/S FREE H2 IN GAS= 7.15589401E-07
H BALANCE CLOSURE = 100.125064 C BALANCE CLOSURE=102.410086

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	5.07592042E-04	1	.164894396
	2	2.03414295E-04	2	.0660803843
	3	5.29436246E-05	3	.0171990619
	4	8.59675573E-04	4	.279270895
	5	0	5	0
	6	6.12972217E-04	6	.199127793
	7	2.5334129E-03	7	0
	8	8.99781267E-04	8	0
	9	7.84482017E-05	9	0
	10	2.88725313E-04	10	.093794193
	11	2.19638546E-04	11	.0713509318
	12	2.53261225E-04	12	.082273466
	13	6.38485767E-04	13	0
	14	8.00627586E-05	14	.0260088793
	H2	.273922709		

KG-MOLE FLUORENE/S IN PRODUCT = 1.66796557E-09
FLUORENE CONVERSION = 42.0433699 %
T-DECALIN CONVERSION= -20.423228 %
C-DECALIN CONVERSION= 72.3720533 %

RUN NUMBER =114 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN114TP
PUMP TEMP/ DEG K =394.816667
INITIAL TIME OF M. B./S =8821.8 FINAL TIME=12502.8
INITIAL PUMP VOL/M3= 1.504E-04 FINAL VOL/M3= 1.6085E-04
WT % OF TRANS-DECALIN =31.127
CIS-DECALIN = 48.187
TETRALIN = 1.088
FLUORENE = 19.599
BAROMETRIC PRESSURE/ BARS =1.0290054
P CORRECTION/ BARS = 4.4018E-03
H20 VAPOR PRESS/ BARS = .04005638
WTM SEC/REV AVERAGE=77.4 WTM TEMP/K=300.927778
KGMS OF CATALYST =7.0013E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=302.038889
KGS/SEC IN COND A=2.2439295E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =593
GC AREA COUNTS, GAS 4 =37879 GAS 5 =70354
GC AREA COUNTS, GAS 6 =14458 GAS 7 =9289

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.065	27	2.784	1	0	27	0
2	.032	28	3.51	2	0	28	0
3	.193	29	32.768	3	0	29	0
4	.39	30	5.711	4	0	30	0
5	.128	31	3	5	0	31	0
6	4.054	32	4.603	6	0	32	0
7	.524	33	1.046	7	0	33	0
8	.227	34	3.257	8	0	34	0
9	1.255	35	.039	9	0	35	0
10	1.066	36	.126	10	0	36	0
11	.215	37	.16	11	0	37	0
12	.038	38	.266	12	0	38	0
13	9E-03	39	.852	13	0	39	0
14	1.365	40	.349	14	0	40	0
15	.141	41	.464	15	0	41	0
16	.084	42	.389	16	0	42	0
17	.071	43	.124	17	0	43	0
18	.129	44	.417	18	0	44	0
19	.252	45	.07	19	0	45	0
20	.667	46	.499	20	0	46	0
21	.497	47	.25	21	0	47	0
22	2.625	48	8.635	22	0	48	0
23	4.819	49	2.065	23	0	49	0
24	1.488	50	2.764	24	0	50	0
25	1.87	51	0	25	0	51	0
26	3.648	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 114 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.47417312E-09	7.56804434E-07
C-DECALIN	8.47444278E-09	1.17159171E-06
TETRALIN	2.0008337E-10	2.64530223E-08
FLUORENE	2.86662518E-09	4.76519103E-07

TOTAL KG-MOLE FED/S = 1.70153245E-08
TOTAL KGS FED/S = 2.43136827E-06
PUMP RATE/ M3/S = 2.83892519E-09
TOTAL KG-ATOMS CARBON= 6.43506084E-04
TOTAL KG-ATOMS HYDROGEN= 1.01570429E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.2951647
WHSV (1/S) LIQ FEED BASIS= 3.47271053E-04
VHSV (1/S) = 2.18377114E-04
TOTAL WHSV (1/S) = 5.52850072E-04
MOLAR GAS DENSITY =.26933805 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.75296818
SUPERFICIAL GAS VELOCITY/ M/S = .0139547601

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.24376795E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.23681921E-07
H2 FEEDRATE KG-MOLE/S = 7.1966595E-07
FRACTION OF GAS THAT IS HYDROCARBONS =4.43446453E-03
KG-MOLE/S FREE H2 IN GAS= 7.20472779E-07
H BALANCE CLOSURE = 99.7631868 C BALANCE CLOSURE=99.6296166

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	1.25122366E-03	1	.269946048
2	5.33988358E-04	2	.115205659
3	1.2597886E-04	3	.0271793896
4	1.04936118E-03	4	.226395097
5	0	5	0
6	5.58973766E-04	6	.120596152
7	1.93354295E-03	7	0
8	3.36989251E-04	8	0
9	6.45411067E-05	9	0
10	5.0210082E-04	10	.108326062
11	3.08513938E-04	11	.0665605365
12	1.79854676E-04	12	.038802862
13	4.23761957E-04	13	0
14	1.2509265E-04	14	.0269881937
H2	.261944127		

KG-MOLE FLUORENE/S IN PRODUCT = 1.16554992E-09
FLUORENE CONVERSION = 59.3406936 %
T-DECALIN CONVERSION= 2.84968628 %
C-DECALIN CONVERSION= 89.0626073 %

RUN NUMBER =115 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN115PR
PUMP TEMP/ DEG K =395.372222
INITIAL TIME OF M. B./S =10773 FINAL TIME=14469.6
INITIAL PUMP VOL/M3= 1.9114E-04 FINAL VOL/M3= 2.0164E-04
WT % OF TRANS-DECALIN =31.127
CIS-DECALIN = 48.187
TETRALIN = 1.088
FLUORENE = 19.599
BAROMETRIC PRESSURE/ BARS =1.0218948
P CORRECTION/ BARS = 4.36794E-03
H20 VAPOR PRESS/ BARS = .03650108
WTM SEC/REV AVERAGE=77.4 WTM TEMP/K=299.816667
KGMS OF CATALYST =7.004E-03 VOLUME/M3=1.28E-05
REACTOR PRESS/BARS=4.4607892 REACTOR TEMP/K=660.761112
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.372223
KGS/SEC IN COND A=2.01149424E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =63
GC AREA COUNTS, GAS 4 =25673 GAS 5 =52933
GC AREA COUNTS, GAS 6 =8108 GAS 7 =8638

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.016	27	1.722	1	0	27	0
2	.016	28	2.99	2	0	28	0
3	.047	29	34.793	3	0	29	0
4	.114	30	12.034	4	0	30	0
5	.036	31	2.931	5	0	31	0
6	1.29	32	5.333	6	0	32	0
7	.035	33	0	7	0	33	0
8	.135	34	3.375	8	0	34	0
9	.344	35	.199	9	0	35	0
10	.341	36	.281	10	0	36	0
11	.069	37	.462	11	0	37	0
12	0	38	0	12	0	38	0
13	0	39	1.417	13	0	39	0
14	.414	40	.753	14	0	40	0
15	.051	41	.408	15	0	41	0
16	.03	42	.451	16	0	42	0
17	.043	43	.192	17	0	43	0
18	.086	44	.595	18	0	44	0
19	.1	45	.289	19	0	45	0
20	.258	46	1	20	0	46	0
21	.247	47	.569	21	0	47	0
22	1.523	48	12.051	22	0	48	0
23	4.097	49	2.637	23	0	49	0
24	0	50	2.208	24	0	50	0
25	1.375	51	0	25	0	51	0
26	2.647	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 115 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.47407418E-09	7.56790756E-07
C-DECALIN	8.47428962E-09	1.17157054E-06
TETRALIN	2.00079753E-10	2.64525442E-08
FLUORENE	2.86657336E-09	4.7651049E-07

TOTAL KG-MOLE FED/S = 1.70150169E-08
TOTAL KGS FED/S = 2.43132433E-06
PUMP RATE/ M3/S = 2.8404707E-09
TOTAL KG-ATOMS CARBON= 6.43494454E-04
TOTAL KG-ATOMS HYDROGEN= 1.01568594E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.3007401
WHSV (1/S) LIQ FEED BASIS= 3.47130908E-04
VHSV (1/S) = 2.21909998E-04
TOTAL WHSV (1/S) = 5.52654053E-04
MOLAR GAS DENSITY =.0811856828 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =1.41047433
SUPERFICIAL GAS VELOCITY/ M/S = .0463008232

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.01134942E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.22032232E-07
H2 FEEDRATE KG-MOLE/S = 7.19747809E-07
FRACTION OF GAS THAT IS HYDROCARBONS =3.16460457E-03
KG-MOLE/S FREE H2 IN GAS= 7.19747286E-07
H BALANCE CLOSURE = 97.4229853 C BALANCE CLOSURE=88.3642911

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	2.58371677E-04	1	.273991581
2	4.5597166E-05	2	.0483537506
3	1.31121894E-05	3	.0139048891
4	1.55653467E-04	4	.165063525
5	0	5	0
6	1.1536023E-04	6	.122334353
7	5.57927231E-04	7	0
8	1.92972618E-04	8	0
9	0	9	0
10	1.52855599E-04	10	.162096511
11	1.07653009E-04	11	.11416119
12	6.72314087E-05	12	.0712958953
13	1.60717994E-04	13	0
14	2.71565513E-05	14	.0287983054
H2	.0793310736		

KG-MOLE FLUORENE/S IN PRODUCT = 1.45814666E-09
FLUORENE CONVERSION = 49.1327633 %
T-DECALIN CONVERSION= 7.52941952 %
C-DECALIN CONVERSION= 79.3400584 %

RUN NUMBER =116 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN116NI
PUMP TEMP/ DEG K =392.594445
INITIAL TIME OF M. B./S =9377.4 FINAL TIME=13114.8
INITIAL PUMP VOL/M3= 3.872E-05 FINAL VOL/M3= 4.935E-05
WT % OF TRANS-DECALIN =31.055
CIS-DECALIN = 47.802
TETRALIN = 1.054
FLUORENE = 20.088
BAROMETRIC PRESSURE/ BARS =1.0097052
P CORRECTION/ BARS = 4.33408E-03
H20 VAPOR PRESS/ BARS = .03822794
WTM SEC/REV AVERAGE=78 WTM TEMP/K=301.483334
KGMS OF CATALYST =7.005E-03 VOLUME/M3=1.32E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.65
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=301.205556
KGS/SEC IN COND A=2.45639094E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =295.372223
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =1838 GAS 5 =4845
GC AREA COUNTS, GAS 6 =1287 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	0	27	0	1	0	27	0
2	0	28	0	2	0	28	0
3	0	29	31.821	3	0	29	0
4	0	30	43.025	4	0	30	0
5	0	31	0	5	0	31	0
6	.079	32	.453	6	0	32	0
7	.034	33	1.153	7	0	33	0
8	0	34	.456	8	0	34	0
9	0	35	0	9	0	35	0
10	.027	36	0	10	0	36	0
11	0	37	0	11	0	37	0
12	0	38	0	12	0	38	0
13	0	39	.033	13	0	39	0
14	.021	40	.095	14	0	40	0
15	0	41	.067	15	0	41	0
16	0	42	.067	16	0	42	0
17	0	43	0	17	0	43	0
18	0	44	0	18	0	44	0
19	0	45	0	19	0	45	0
20	.05	46	.128	20	0	46	0
21	9E-03	47	0	21	0	47	0
22	.138	48	20.079	22	0	48	0
23	.375	49	.803	23	0	49	0
24	0	50	.492	24	0	50	0
25	.261	51	0	25	0	51	0
26	.341	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 116 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.49063113E-09	7.59079753E-07
C-DECALIN	8.4515585E-09	1.16842796E-06
TETRALIN	1.94864254E-10	2.57630031E-08
FLUORENE	2.95381417E-09	4.91012529E-07

TOTAL KG-MOLE FED/S = 1.7090868E-08
TOTAL KGS FED/S = 2.44428325E-06
PUMP RATE/ M3/S = 2.84424601E-09
TOTAL KG-ATOMS CARBON= 6.47167266E-04
TOTAL KG-ATOMS HYDROGEN= 1.01820119E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 40.9700858
WHSV (1/S) LIQ FEED BASIS= 3.48931291E-04
VHSV (1/S) = 2.15471459E-04
TOTAL WHSV (1/S) = 5.4884813E-04
MOLAR GAS DENSITY =.269451265 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.9585381
SUPERFICIAL GAS VELOCITY/ M/S = .013582015

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.45621409E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.02097359E-07
H2 FEEDRATE KG-MOLE/S = 7.00214329E-07
FRACTION OF GAS THAT IS HYDROCARBONS =2.66557772E-04
KG-MOLE/S FREE H2 IN GAS= 7.0191021E-07
H BALANCE CLOSURE = 100.138877 C BALANCE CLOSURE=101.08133

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	7.01101382E-05	1	.213924444
2	8.63733407E-06	2	.0263547747
3	2.53020003E-06	3	7.7203048E-03
4	4.78862889E-05	4	.146113644
5	0	5	0
6	4.23302008E-05	6	.12916056
7	2.11790773E-03	7	0
8	2.86361146E-03	8	0
9	8.02459929E-05	9	0
10	3.15276971E-05	10	.096199284
11	4.10143755E-05	11	.125145631
12	5.85810765E-05	12	.17874625
13	1.11145281E-03	13	0
14	2.51158674E-05	14	.0766351077
H2	.262950314		

KG-MOLE FLUORENE/S IN PRODUCT = 2.96687257E-09
FLUORENE CONVERSION = -.442086277 %
T-DECALIN CONVERSION= -2.96571388 %
C-DECALIN CONVERSION= 9.55487645 %

RUN NUMBER =117.1 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN117ACT-1
PUMP TEMP/ DEG K =394.261111
INITIAL TIME OF M. B./S =11802.6 FINAL TIME=15546.6
INITIAL PUMP VOL/M3= 8.335E-05 FINAL VOL/M3= 9.399E-05
WT % OF TRANS-DECALIN =31.055
CIS-DECALIN = 47.802
TETRALIN = 1.054
FLUORENE = 20.088
BAROMETRIC PRESSURE/ BARS =1.0252808
P CORRECTION/ BARS = 4.4018E-03
H20 VAPOR PRESS/ BARS = .03565458
WTM SEC/REV AVERAGE=79.2 WTM TEMP/K=302.038889
KGMS OF CATALYST =7.0308E-03 VOLUME/M3=1.32E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=633.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=302.316667
KGS/SEC IN COND A=2.25006888E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =298.15
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =539
GC AREA COUNTS, GAS 4 =17564 GAS 5 =31490
GC AREA COUNTS, GAS 6 =6425 GAS 7 =3599

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.024	27	.836	1	0	27	0
2	9E-03	28	3.411	2	0	28	0
3	.014	29	41.791	3	0	29	0
4	0	30	14.559	4	0	30	0
5	0	31	1.963	5	0	31	0
6	.315	32	2.963	6	0	32	0
7	.065	33	1.361	7	0	33	0
8	0	34	2.198	8	0	34	0
9	.132	35	.054	9	0	35	0
10	.177	36	.07	10	0	36	0
11	.031	37	.074	11	0	37	0
12	0	38	.213	12	0	38	0
13	0	39	.685	13	0	39	0
14	.177	40	.275	14	0	40	0
15	.038	41	.436	15	0	41	0
16	.021	42	.439	16	0	42	0
17	.022	43	.072	17	0	43	0
18	.064	44	.362	18	0	44	0
19	.061	45	.147	19	0	45	0
20	.111	46	.548	20	0	46	0
21	.132	47	.197	21	0	47	0
22	1.06	48	13.575	22	0	48	0
23	3.177	49	2.709	23	0	49	0
24	0	50	2.439	24	0	50	0
25	.462	51	0	25	0	51	0
26	2.533	52	0	26	0	52	0
		53	0			53	0

```
RUN NUMBER  117.1   MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES
COMPOUND          KG-MOLE/SECOND          KG/S
T-DECALIN      5.47690186E-09          7.57181682E-07
C-DECALIN      8.43042547E-09          1.16550632E-06
TETRALIN      1.94376998E-10          2.56985829E-08
FLUORENE      2.94642818E-09          4.89784757E-07
TOTAL KG-MOLE FED/S =  1.70481325E-08
TOTAL   KGS FED/S =  2.43817134E-06
PUMP RATE/ M3/S  =  2.84190308E-09
TOTAL KG-ATOMS CARBON=   6.4554903E-04
TOTAL KG-ATOMS HYDROGEN=   1.01565519E-03


FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.1309676
WHSV (1/S) LIQ FEED BASIS=  3.46781567E-04
VHSV (1/S) =       2.15293965E-04
TOTAL WHSV (1/S) = 5.46246941E-04
MOLAR GAS DENSITY =.280806273  KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC    =5.16066852
SUPERFICIAL GAS VELOCITY/  M/S   =    .0130500416


MATERIAL BALANCE CLOSURE RESULTS
  KGS/S  IN COND A= 2.24990689E-06   KGS/S IN COND B= 0
KG-MOLE/S  OF ALL GAS OUT= 7.11340168E-07
H2 FEEDRATE KG-MOLE/S  = 7.01206186E-07
FRACTION OF GAS THAT IS HYDROCARBONS =2.00512879E-03
KG-MOLE/S FREE H2 IN GAS=  7.09913839E-07
H BALANCE CLOSURE = 99.68353  C BALANCE CLOSURE=95.8884964
                    PRODUCT DISTRIBUTION
          WITH FEEDSTOCK                WITHOUT FEEDSTOCK
COMPOUND GROUP CONC./KG-MOLE/M3   COMP. GROUP   MOLE FRAC.
       1       5.57263581E-04         1       .232342745
       2       5.35086924E-05         2       .0223096518
       3       2.03016467E-05         3       8.464469E-03
       4       5.54951589E-04         4       .231378794
       5       0                      5       0
       6       2.81155293E-04         6       .117223509
       7       2.62564489E-03         7       0
       8       9.1471283E-04          8       0
       9       8.94153714E-05         9       0
       10      3.48046255E-04         10      .145112699
       11      2.40148593E-04         11      .100126377
       12      2.25547526E-04         12      .0940386794
       13      7.09330768E-04         13      0
       14      1.17531666E-04         14      .0490030764
       H2      .274068714
KG-MOLE FLUORENE/S  IN PRODUCT =  1.837363055-09
FLUORENE CONVERSION =  37.6410035  %
T-DECALIN CONVERSION=  -24.1787288  %
C-DECALIN CONVERSION=  71.895138  %
```

RUN NUMBER =117.2 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN117ACT-2
PUMP TEMP/ DEG K =394.261111
INITIAL TIME OF M. B./S =24211.8 FINAL TIME=28003.2
INITIAL PUMP VOL/M3= 1.1861E-04 FINAL VOL/M3= 1.2938E-04
WT % OF TRANS-DECALIN =31.055
CIS-DECALIN = 47.802
TETRALIN = 1.054
FLUORENE = 20.088
BAROMETRIC PRESSURE/ BARS =1.0252808
P CORRECTION/ BARS = 4.4018E-03
H20 VAPOR PRESS/ BARS = .03565458
WTM SEC/REV AVERAGE=79.2 WTM TEMP/K=301.483334
KGMS OF CATALYST =7.0308E-03 VOLUME/M3=1.32E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=633.983334
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=300.372223
KGS/SEC IN COND A=2.33335332E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.594445
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =10982 GAS 5 =20385
GC AREA COUNTS, GAS 6 =3362 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.017	27	.898	1	0	27	0
2	0	28	2.965	2	0	28	0
3	.024	29	36.887	3	0	29	0
4	.053	30	22.887	4	0	30	0
5	.017	31	1.133	5	0	31	0
6	.921	32	1.651	6	0	32	0
7	0	33	.974	7	0	33	0
8	.01	34	1.459	8	0	34	0
9	.293	35	.018	9	0	35	0
10	.319	36	.04	10	0	36	0
11	.057	37	0	11	0	37	0
12	0	38	.089	12	0	38	0
13	0	39	.268	13	0	39	0
14	.283	40	.112	14	0	40	0
15	.058	41	.386	15	0	41	0
16	.032	42	.344	16	0	42	0
17	.037	43	0	17	0	43	0
18	.088	44	.28	18	0	44	0
19	.065	45	.16	19	0	45	0
20	.133	46	.402	20	0	46	0
21	.113	47	.138	21	0	47	0
22	1.024	48	13.993	22	0	48	0
23	3.543	49	2.242	23	0	49	0
24	0	50	1.671	24	0	50	0
25	1.251	51	0	25	0	51	0
26	2.669	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 117.2 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.47451019E-09	7.56851033E-07
C-DECALIN	8.42674404E-09	1.16499736E-06
TETRALIN	1.94292117E-10	2.56873608E-08
FLUORENE	2.94514153E-09	4.89570876E-07

TOTAL KG-MOLE FED/S = 1.70406879E-08
TOTAL KGS FED/S = 2.43710664E-06
PUMP RATE/ M3/S = 2.84066206E-09
TOTAL KG-ATOMS CARBON= 6.4526713E-04
TOTAL KG-ATOMS HYDROGEN= 1.01521167E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.2247174
WHSV (1/S) LIQ FEED BASIS= 3.46630133E-04
VHSV (1/S) = 2.1519995E-04
TOTAL WHSV (1/S) = 5.46462847E-04
MOLAR GAS DENSITY =.280781673 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =5.15100878
SUPERFICIAL GAS VELOCITY/ M/S = .0130745145

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.33318533E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.06991489E-07
H2 FEEDRATE KG-MOLE/S = 7.02497542E-07
FRACTION OF GAS THAT IS HYDROCARBONS =1.17982088E-03
KG-MOLE/S FREE H2 IN GAS= 7.06157367E-07
H BALANCE CLOSURE = 99.7042389 C BALANCE CLOSURE=97.8121923
PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	3.36625655E-04	1	.162509647
	2	1.41006492E-04	2	.0680723972
	3	3.81469626E-05	3	.0184158555
	4	5.55759811E-04	4	.268299012
	5	0	5	0
	6	3.726894E-04	6	.179919807
	7	2.41521326E-03	7	0
	8	1.49854924E-03	8	0
	9	6.66871167E-05	9	0
	10	1.99713835E-04	10	.0964139967
	11	1.52709979E-04	11	.0737223812
	12	1.90850671E-04	12	.0921352095
	13	7.61989028E-04	13	0
	14	8.39167133E-05	14	.0405116938
	H2	.273967815		

KG-MOLE FLUORENE/S IN PRODUCT = 1.96404153E-09
FLUORENE CONVERSION = 33.3124908 %
T-DECALIN CONVERSION= -13.7135361 %
C-DECALIN CONVERSION= 54.1633188 %

RUN NUMBER =117.3 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN117ACT-3
PUMP TEMP/ DEG K =394.261111
INITIAL TIME OF M. B./S =38047.2 FINAL TIME=41866.8
INITIAL PUMP VOL/M3= 1.5791E-04 FINAL VOL/M3= 1.6875E-04
WT % OF TRANS-DECALIN =31.055
CIS-DECALIN = 47.802
TETRALIN = 1.054
FLUORENE = 20.088
BAROMETRIC PRESSURE/ BARS =1.0252808
P CORRECTION/ BARS = 4.4018E-03
H20 VAPOR PRESS/ BARS = .03565458
WTM SEC/REV AVERAGE=79.8 WTM TEMP/K=299.816667
KGMS OF CATALYST =7.0308E-03 VOLUME/M3=1.32E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=633.927778
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=299.677778
KGS/SEC IN COND A=2.31274056E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =8311 GAS 5 =15412
GC AREA COUNTS, GAS 6 =3285 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.01	27	.513	1	0	27	0
2	0	28	1.929	2	0	28	0
3	0	29	35.834	3	0	29	0
4	0	30	31.264	4	0	30	0
5	0	31	.694	5	0	31	0
6	.13	32	1.138	6	0	32	0
7	0	33	.906	7	0	33	0
8	.026	34	1.196	8	0	34	0
9	.048	35	.011	9	0	35	0
10	.074	36	.022	10	0	36	0
11	0	37	.011	11	0	37	0
12	0	38	.051	12	0	38	0
13	0	39	.181	13	0	39	0
14	.068	40	.067	14	0	40	0
15	.015	41	.281	15	0	41	0
16	0	42	.269	16	0	42	0
17	0	43	0	17	0	43	0
18	.04	44	.174	18	0	44	0
19	.02	45	.156	19	0	45	0
20	.037	46	.31	20	0	46	0
21	.043	47	.113	21	0	47	0
22	.675	48	15.691	22	0	48	0
23	1.876	49	2.039	23	0	49	0
24	0	50	1.28	24	0	50	0
25	1.085	51	0	25	0	51	0
26	1.725	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 117.3 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.46941114E-09	7.5614609E-07
C-DECALIN	8.41889523E-09	1.16391227E-06
TETRALIN	1.9411115E-10	2.56634352E-08
FLUORENE	2.94239838E-09	4.89114882E-07

TOTAL KG-MOLE FED/S = 1.70248159E-08
TOTAL KGS FED/S = 2.43483667E-06
PUMP RATE/ M3/S = 2.83801622E-09
TOTAL KG-ATOMS CARBON= 6.44666117E-04
TOTAL KG-ATOMS HYDROGEN= 1.01426608E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.1804174
WHSV (1/S) LIQ FEED BASIS= 3.46307276E-04
VHSV (1/S) = 2.14999509E-04
TOTAL WHSV (1/S) = 5.45739323E-04
MOLAR GAS DENSITY =.280806273 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =5.16167805
SUPERFICIAL GAS VELOCITY/ M/S = .0130474892

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.31257405E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.03397018E-07
H2 FEEDRATE KG-MOLE/S = 7.01089025E-07
FRACTION OF GAS THAT IS HYDROCARBONS =9.16108627E-04
KG-MOLE/S FREE H2 IN GAS= 7.0275263E-07
H BALANCE CLOSURE = 99.3441929 C BALANCE CLOSURE=96.5869159

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	2.52965429E-04	1	.19033929
	2	2.15639529E-05	2	.0162254087
	3	1.0793331E-05	3	8.12124791E-03
	4	3.40135669E-04	4	.25592897
	5	0	5	0
	6	2.26725843E-04	6	.170595785
	7	2.33865684E-03	7	0
	8	2.04040206E-03	8	0
	9	6.18301419E-05	9	0
	10	1.30887688E-04	10	.098484088
	11	1.18975025E-04	11	.089520619
	12	1.62904364E-04	12	.12257446
	13	8.51682195E-04	13	0
	14	6.40724081E-05	14	.0482101317
	H2	.274184678		

KG-MOLE FLUORENE/S IN PRODUCT = 2.18291521E-09
FLUORENE CONVERSION = 25.8117043 %
T-DECALIN CONVERSION= -9.59360863 %
C-DECALIN CONVERSION= 37.881645 %

RUN NUMBER =117.4 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN117ACT-4
PUMP TEMP/ DEG K =394.261111
INITIAL TIME OF M. B./S =52834.8 FINAL TIME=56677.2
INITIAL PUMP VOL/M3= 1.999E-04 FINAL VOL/M3= 2.108E-04
WT % OF TRANS-DECALIN =31.055
CIS-DECALIN = 47.802
TETRALIN = 1.054
FLUORENE = 20.088
BAROMETRIC PRESSURE/ BARS =1.0252808
P CORRECTION/ BARS = 4.4018E-03
H20 VAPOR PRESS/ BARS = .03565458
WTM SEC/REV AVERAGE=80.4 WTM TEMP/K=298.427778
KGMS OF CATALYST =7.0308E-03 VOLUME/M3=1.32E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=633.816667
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=298.427778
KGS/SEC IN COND A=2.28659958E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =295.927778
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =6737 GAS 5 =12321
GC AREA COUNTS, GAS 6 =2260 GAS 7 =2163

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	8E-03	27	.343	1	0	27	0
2	0	28	1.285	2	0	28	0
3	0	29	34.421	3	0	29	0
4	0	30	36.458	4	0	30	0
5	0	31	.816	5	0	31	0
6	.136	32	0	6	0	32	0
7	0	33	.86	7	0	33	0
8	.034	34	1.011	8	0	34	0
9	.045	35	0	9	0	35	0
10	.065	36	0	10	0	36	0
11	0	37	.026	11	0	37	0
12	0	38	.048	12	0	38	0
13	0	39	.168	13	0	39	0
14	.056	40	.063	14	0	40	0
15	9E-03	41	.248	15	0	41	0
16	0	42	.227	16	0	42	0
17	0	43	0	17	0	43	0
18	.042	44	.131	18	0	44	0
19	.017	45	.156	19	0	45	0
20	.033	46	.238	20	0	46	0
21	.029	47	.098	21	0	47	0
22	.46	48	16.49	22	0	48	0
23	1.277	49	1.794	23	0	49	0
24	0	50	.992	24	0	50	0
25	.752	51	0	25	0	51	0
26	1.167	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 117.4 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.46705062E-09	7.55819748E-07
C-DECALIN	8.41526176E-09	1.16340994E-06
TETRALIN	1.94027375E-10	2.56523592E-08
FLUORENE	2.94112848E-09	4.88903787E-07

TOTAL KG-MOLE FED/S = 1.70174682E-08
TOTAL KGS FED/S = 2.43378583E-06
PUMP RATE/ M3/S = 2.83679138E-09
TOTAL KG-ATOMS CARBON= 6.44387889E-04
TOTAL KG-ATOMS HYDROGEN= 1.01382834E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.0809383
WHSV (1/S) LIQ FEED BASIS= 3.46157815E-04
VHSV (1/S) = 2.14906719E-04
TOTAL WHSV (1/S) = 5.45022231E-04
MOLAR GAS DENSITY =.280855485 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =5.1770213
SUPERFICIAL GAS VELOCITY/ M/S = .0130088201

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.28643496E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.02150183E-07
H2 FEEDRATE KG-MOLE/S = 6.99093562E-07
FRACTION OF GAS THAT IS HYDROCARBONS =7.80903528E-04
KG-MOLE/S FREE H2 IN GAS= 7.01601872E-07
H BALANCE CLOSURE = 99.3487014 C BALANCE CLOSURE=95.2880027

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	2.15636241E-04	1	.220063891
2	2.18913908E-05	2	.0223408857
3	1.02475137E-05	3	.0104579254
4	2.28702143E-04	4	.233398074
5	0	5	0
6	1.5339724E-04	6	.156546939
7	2.22600607E-03	7	0
8	2.35773886E-03	8	0
9	5.81570203E-05	9	0
10	5.97065872E-05	10	.0609325399
11	1.01460372E-04	11	.103543653
12	1.39634225E-04	12	.142501328
13	8.86909388E-04	13	0
14	4.9204452E-05	14	.0502147648
H2	.274346794		

KG-MOLE FLUORENE/S IN PRODUCT = 2.26814128E-09
FLUORENE CONVERSION = 22.8819383 %
T-DECALIN CONVERSION= -4.12717828 %
C-DECALIN CONVERSION= 28.3495499 %

RUN NUMBER =117.5 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN117ACT-5
PUMP TEMP/ DEG K =394.261111
INITIAL TIME OF M. B./S =62323.2 FINAL TIME=66165
INITIAL PUMP VOL/M3= 2.2684E-04 FINAL VOL/M3= 2.3775E-04
WT % OF TRANS-DECALIN =31.055
CIS-DECALIN = 47.802
TETRALIN = 1.054
FLUORENE = 20.088
BAROMETRIC PRESSURE/ BARS =1.0252808
P CORRECTION/ BARS = 4.4018E-03
H20 VAPOR PRESS/ BARS = .03565458
WTM SEC/REV AVERAGE=80.4 WTM TEMP/K=298.705556
KGMS OF CATALYST =7.0308E-03 VOLUME/M3=1.32E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=633.983334
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=298.705556
KGS/SEC IN COND A=2.38460742E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =295.372223
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =0
GC AREA COUNTS, GAS 4 =6473 GAS 5 =10990
GC AREA COUNTS, GAS 6 =3107 GAS 7 =0

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	7E-03	27	.286	1	0	27	0
2	0	28	1.086	2	0	28	0
3	6E-03	29	33.24	3	0	29	0
4	.017	30	38.017	4	0	30	0
5	0	31	.664	5	0	31	0
6	.431	32	0	6	0	32	0
7	.087	33	.844	7	0	33	0
8	0	34	.931	8	0	34	0
9	.13	35	0	9	0	35	0
10	.146	36	.065	10	0	36	0
11	.023	37	0	11	0	37	0
12	0	38	.049	12	0	38	0
13	0	39	.146	13	0	39	0
14	.125	40	.052	14	0	40	0
15	.025	41	.252	15	0	41	0
16	.013	42	.218	16	0	42	0
17	.011	43	.128	17	0	43	0
18	.073	44	0	18	0	44	0
19	.026	45	0	19	0	45	0
20	.05	46	.097	20	0	46	0
21	.045	47	0	21	0	47	0
22	.466	48	16.936	22	0	48	0
23	1.02	49	1.71	23	0	49	0
24	0	50	.988	24	0	50	0
25	.637	51	0	25	0	51	0
26	.954	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 117.5 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.47292091E-09	7.56631315E-07
C-DECALIN	8.42429771E-09	1.16465916E-06
TETRALIN	1.94235713E-10	2.56799036E-08
FLUORENE	2.94428654E-09	4.89428751E-07

TOTAL KG-MOLE FED/S = 1.70357409E-08
TOTAL KGS FED/S = 2.43639913E-06
PUMP RATE/ M3/S = 2.8398374E-09
TOTAL KG-ATOMS CARBON= 6.45079805E-04
TOTAL KG-ATOMS HYDROGEN= 1.01491695E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 40.9987363
WHSV (1/S) LIQ FEED BASIS= 3.46529504E-04
VHSV (1/S) = 2.15137476E-04
TOTAL WHSV (1/S) = 5.45209103E-04
MOLAR GAS DENSITY =.280781673 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =5.18022848
SUPERFICIAL GAS VELOCITY/ M/S = .0130007661

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.38443574E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.0160719E-07
H2 FEEDRATE KG-MOLE/S = 6.98443847E-07
FRACTION OF GAS THAT IS HYDROCARBONS =6.98613536E-04
KG-MOLE/S FREE H2 IN GAS= 7.01117038E-07
H BALANCE CLOSURE = 100.005091 C BALANCE CLOSURE=99.0534165
PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	1.95294792E-04	1	.203055122
	2	6.93851925E-05	2	.0721423164
	3	1.68456319E-05	3	.0175150182
	4	2.27938358E-04	4	.236995829
	5	0	5	0
	6	1.30968192E-04	6	.136172408
	7	2.24054694E-03	7	0
	8	2.5625413E-03	8	0
	9	5.94889513E-05	9	0
	10	5.40675761E-05	10	.0562160318
	11	8.88114769E-05	11	.0923405333
	12	1.27392232E-04	12	.132454353
	13	9.49422702E-04	13	0
	14	5.10787009E-05	14	.0531083892
	H2	.274007891		

KG-MOLE FLUORENE/S IN PRODUCT = 2.42933308E-09
FLUORENE CONVERSION = 17.4899235 %
T-DECALIN CONVERSION= -4.75200064 %
C-DECALIN CONVERSION= 22.1668478 %

RUN NUMBER =118 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN118DIF
PUMP TEMP/ DEG K =393.705556
INITIAL TIME OF M. B./S =8749.8 FINAL TIME=12451.2
INITIAL PUMP VOL/M3= 3.643E-05 FINAL VOL/M3= 4.694E-05
WT % OF TRANS-DECALIN =30.417
CIS-DECALIN = 47.376
TETRALIN = 1.096
FLUORENE = 21.11
BAROMETRIC PRESSURE/ BARS =1.025958
P CORRECTION/ BARS = 4.77426E-03
H20 VAPOR PRESS/ BARS = .03914216
WTM SEC/REV AVERAGE=77.4 WTM TEMP/K=300.927778
KGMS OF CATALYST =7.0013E-03 VOLUME/M3=1.3E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.15
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=301.483334
KGS/SEC IN COND A=2.43066666E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =297.038889
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =724
GC AREA COUNTS, GAS 4 =23350 GAS 5 =46126
GC AREA COUNTS, GAS 6 =8663 GAS 7 =7656

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	7E-03	27	1.713	1	0	27	0
2	.044	28	3.311	2	0	28	0
3	.131	29	33.606	3	0	29	0
4	.268	30	12.8	4	0	30	0
5	.085	31	2.108	5	0	31	0
6	2.889	32	3.192	6	0	32	0
7	.355	33	.989	7	0	33	0
8	.213	34	2.317	8	0	34	0
9	.841	35	.163	9	0	35	0
10	.749	36	.131	10	0	36	0
11	.148	37	.229	11	0	37	0
12	.026	38	0	12	0	38	0
13	9E-03	39	.658	13	0	39	0
14	.784	40	.332	14	0	40	0
15	.103	41	.798	15	0	41	0
16	.061	42	.673	16	0	42	0
17	.066	43	.244	17	0	43	0
18	.133	44	.684	18	0	44	0
19	.161	45	.021	19	0	45	0
20	.379	46	.279	20	0	46	0
21	.341	47	.14	21	0	47	0
22	2.46	48	11.512	22	0	48	0
23	4.77	49	2.238	23	0	49	0
24	0	50	2.075	24	0	50	0
25	1.638	51	0	25	0	51	0
26	3.128	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 118 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.37727561E-09	7.43408353E-07
C-DECALIN	8.37537592E-09	1.15789572E-06
TETRALIN	2.02608335E-10	2.6786848E-08
FLUORENE	3.10377254E-09	5.1594011E-07

TOTAL KG-MOLE FED/S = 1.70590324E-08
TOTAL KGS FED/S = 2.44403103E-06
PUMP RATE/ M3/S = 2.83948887E-09
TOTAL KG-ATOMS CARBON= 6.47640729E-04
TOTAL KG-ATOMS HYDROGEN= 1.01165222E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.0794338
WHSV (1/S) LIQ FEED BASIS= 3.49079668E-04
VHSV (1/S) = 2.18420473E-04
TOTAL WHSV (1/S) = 5.54135495E-04
MOLAR GAS DENSITY =.269655292 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.77014294
SUPERFICIAL GAS VELOCITY/ M/S = .0139045164

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.43049167E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.19183833E-07
H2 FEEDRATE KG-MOLE/S = 7.17834424E-07
FRACTION OF GAS THAT IS HYDROCARBONS =2.8817015E-03
KG-MOLE/S FREE H2 IN GAS= 7.1711136E-07
H BALANCE CLOSURE = 100.306108 C BALANCE CLOSURE=104.3012

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	8.18391388E-04	1	.221476584
	2	4.12849605E-04	2	.111727129
	3	1.03699818E-04	3	.0280636891
	4	8.48016742E-04	4	.229493925
	5	0	5	0
	6	5.22203952E-04	6	.141321071
	7	2.16096368E-03	7	0
	8	8.23077279E-04	8	0
	9	6.65009378E-05	9	0
	10	3.88174604E-04	10	.105049475
	11	2.77523667E-04	11	.0751046439
	12	2.21961703E-04	12	.0600682273
	13	6.15654643E-04	13	0
	14	1.02338397E-04	14	.0276952556
	H2	.262293935		

KG-MOLE FLUORENE/S IN PRODUCT = 1.68319919E-09
FLUORENE CONVERSION = 45.7692481 %
T-DECALIN CONVERSION= -9.87111292 %
C-DECALIN CONVERSION= 73.1320422 %

RUN NUMBER =119 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN119DIF
PUMP TEMP/ DEG K =394.594445
INITIAL TIME OF M. B./S =9168.6 FINAL TIME=12804
INITIAL PUMP VOL/M3= 8.892E-05 FINAL VOL/M3= 1.0545E-04
WT % OF TRANS-DECALIN =30.417
CIS-DECALIN = 47.376
TETRALIN = 1.096
FLUORENE = 21.11
BAROMETRIC PRESSURE/ BARS =1.0218948
P CORRECTION/ BARS = 4.7404E-03
H20 VAPOR PRESS/ BARS = .049733568
WTM SEC/REV AVERAGE=51 WTM TEMP/K=305.094445
KGMS OF CATALYST =.0113082 VOLUME/M3=2.18E-05
REACTOR PRESS/BARS=15.1480392 REACTOR TEMP/K=660.65
INITIAL WTM M3 = 0 FINAL M3 = .101952
WTM TEMP/DEG K DURING M.B.=305.927778
KGS/SEC IN COND A=3.63692982E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =303.15
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =2902
GC AREA COUNTS, GAS 4 =38987 GAS 5 =64586
GC AREA COUNTS, GAS 6 =14449 GAS 7 =7752

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.06	27	2.638	1	0	27	0
2	.039	28	3.746	2	0	28	0
	.146	29	32.937	3	0	29	0
4	.284	30	7.54	4	0	30	0
5	.093	31	2.748	5	0	31	0
6	3.203	32	4.242	6	0	32	0
7	.481	33	.983	7	0	33	0
8	.246	34	3.177	8	0	34	0
9	1.097	35	.037	9	0	35	0
10	.981	36	.103	10	0	36	0
11	.218	37	.118	11	0	37	0
12	.038	38	.208	12	0	38	0
13	0	39	.781	13	0	39	0
14	1.193	40	.316	14	0	40	0
15	.146	41	.426	15	0	41	0
16	.086	42	.394	16	0	42	0
17	.079	43	.105	17	0	43	0
18	.132	44	.406	18	0	44	0
19	.266	45	.065	19	0	45	0
20	.737	46	.532	20	0	46	0
21	.512	47	.252	21	0	47	0
22	2.564	48	8.813	22	0	48	0
23	4.771	49	2.222	23	0	49	0
24	1.314	50	2.826	24	0	50	0
25	1.911	51	0	25	0	51	0
26	3.789	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 119 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	8.60309571E-09	1.18937798E-06
C-DECALIN	1.33997522E-08	1.85251574E-06
TETRALIN	3.24152791E-10	4.28562405E-08
FLUORENE	4.96572134E-09	8.25451859E-07

TOTAL KG-MOLE FED/S = 2.7292722E-08
TOTAL KGS FED/S = 3.91020182E-06
PUMP RATE/ M3/S = 4.54699131E-09
TOTAL KG-ATOMS CARBON= 1.03615949E-03
TOTAL KG-ATOMS HYDROGEN= 1.61854096E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 38.7851399
WHSV (1/S) LIQ FEED BASIS= 3.4578187E-04
VHSV (1/S) = 2.08575915E-04
TOTAL WHSV (1/S) = 5.32998858E-04
MOLAR GAS DENSITY =.275726329 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =5.53567348
SUPERFICIAL GAS VELOCITY/ M/S = .020092314

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 3.63666798E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 1.06629846E-06
H2 FEEDRATE KG-MOLE/S = 1.05855204E-06
FRACTION OF GAS THAT IS HYDROCARBONS =4.36241506E-03
KG-MOLE/S FREE H2 IN GAS= 1.06164682E-06
H BALANCE CLOSURE = 99.9547742 C BALANCE CLOSURE=99.4540268

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	1.24683812E-03	1	.255974021
	2	4.92573908E-04	2	.101124695
	3	1.36764169E-04	3	.0280774816
	4	1.17643868E-03	4	.241521121
	5	0	5	0
	6	6.17999886E-04	6	.126874462
	7	2.18401955E-03	7	0
	8	4.99969864E-04	8	0
	9	6.81595689E-05	9	0
	10	5.13892588E-04	10	.105501388
	11	3.32136093E-04	11	.0681870485
	12	2.10586536E-04	12	.0432331043
	13	4.8601759E-04	13	0
	14	1.43725724E-04	14	.0295066786
	H2	.267617207		

KG-MOLE FLUORENE/S IN PRODUCT = 1.92804878E-09
FLUORENE CONVERSION = 61.1728358 %
T-DECALIN CONVERSION= -.708887512 %
C-DECALIN CONVERSION= 85.1982491 %

RUN NUMBER =120 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN120DIF
PUMP TEMP/ DEG K =395.927778
INITIAL TIME OF M. B./S =8900.4 FINAL TIME=12492.6
INITIAL PUMP VOL/M3= 1.3016E-04 FINAL VOL/M3= 1.4037E-04
WT % OF TRANS-DECALIN =30.417
CIS-DECALIN = 47.376
TETRALIN = 1.096
FLUORENE = 21.11
BAROMETRIC PRESSURE/ BARS =1.024265
P CORRECTION/ BARS = 4.67268E-03
H20 VAPOR PRESS/ BARS = .0386004
WTM SEC/REV AVERAGE=75.9 WTM TEMP/K=300.927778
KGMS OF CATALYST =7.0096E-03 VOLUME/M3=1.28E-05
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=633.038889
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=301.483334
KGS/SEC IN COND A=2.27707104E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =298.15
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =197
GC AREA COUNTS, GAS 4 =12428 GAS 5 =27638
GC AREA COUNTS, GAS 6 =4627 GAS 7 =4288

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.017	27	1.232	1	0	27	0
2	0	28	4.58	2	0	28	0
3	.013	29	37.727	3	0	29	0
4	.06	30	11.622	4	0	30	0
5	.02	31	1.622	5	0	31	0
6	1.057	32	2.398	6	0	32	0
7	.215	33	1.261	7	0	33	0
8	0	34	1.595	8	0	34	0
9	.393	35	.026	9	0	35	0
10	.436	36	.053	10	0	36	0
11	.088	37	.044	11	0	37	0
12	0	38	.118	12	0	38	0
13	0	39	.292	13	0	39	0
14	.329	40	.111	14	0	40	0
15	.083	41	.337	15	0	41	0
16	.043	42	.369	16	0	42	0
17	.06	43	0	17	0	43	0
18	.101	44	.336	18	0	44	0
19	.089	45	.156	19	0	45	0
20	.157	46	.427	20	0	46	0
21	.205	47	.152	21	0	47	0
22	2.383	48	12.715	22	0	48	0
23	6.07	49	2.483	23	0	49	0
24	0	50	1.935	24	0	50	0
25	2.141	51	0	25	0	51	0
26	4.45	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 120 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.37043828E-09	7.42463092E-07
C-DECALIN	8.36472644E-09	1.15642343E-06
TETRALIN	2.02350714E-10	2.67527879E-08
FLUORENE	3.09982603E-09	5.1528408E-07

TOTAL KG-MOLE FED/S = 1.70373415E-08
TOTAL KGS FED/S = 2.44092339E-06
PUMP RATE/ M3/S = 2.84229211E-09
TOTAL KG-ATOMS CARBON= 6.46817239E-04
TOTAL KG-ATOMS HYDROGEN= 1.01036588E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 42.9197509
WHSV (1/S) LIQ FEED BASIS= 3.48222989E-04
VHSV (1/S) = 2.22052295E-04
TOTAL WHSV (1/S) = 5.56860458E-04
MOLAR GAS DENSITY =.281200456 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.81025133
SUPERFICIAL GAS VELOCITY/ M/S = .013576447

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.2769071E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.40254374E-07
H2 FEEDRATE KG-MOLE/S = 7.31238451E-07
FRACTION OF GAS THAT IS HYDROCARBONS =1.62971271E-03
KG-MOLE/S FREE H2 IN GAS= 7.39047972E-07
H BALANCE CLOSURE = 99.8892841 C BALANCE CLOSURE=96.2862852

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	4.60111716E-04	1	.161635789
2	1.58555719E-04	2	.0557001218
3	4.83473618E-05	3	.0169842751
4	8.92795414E-04	4	.313636202
5	0	5	0
6	5.77866792E-04	6	.203002774
7	2.30871338E-03	7	0
8	7.11211252E-04	8	0
9	8.06925925E-05	9	0
10	2.71188773E-04	10	.0952677571
11	1.55885984E-04	11	.0547622526
12	1.91022302E-04	12	.0671055299
13	6.47127487E-04	13	0
14	9.08214818E-05	14	.031905299
H2	.274606115		

KG-MOLE FLUORENE/S IN PRODUCT = 1.74161546E-09
FLUORENE CONVERSION = 43.815703 %
T-DECALIN CONVERSION= -15.6971643 %
C-DECALIN CONVERSION= 77.1171928 %

RUN NUMBER =121 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN121DIF
PUMP TEMP/ DEG K =394.816667
INITIAL TIME OF M. B./S =20388 FINAL TIME=27739.8
INITIAL PUMP VOL/M3= 1.6908E-04 FINAL VOL/M3= 1.7953E-04
WT % OF TRANS-DECALIN =30.417
CIS-DECALIN = 47.376
TETRALIN = 1.096
FLUORENE = 21.11
BAROMETRIC PRESSURE/ BARS =1.0127526
P CORRECTION/ BARS = 4.9097E-03
H20 VAPOR PRESS/ BARS = .03399544
WTM SEC/REV AVERAGE=146.7 WTM TEMP/K=299.261111
KGMS OF CATALYST =3.5608E-03 VOLUME/M3=6.7E-06
REACTOR PRESS/BARS=14.8032892 REACTOR TEMP/K=660.983334
INITIAL WTM M3 = 0 FINAL M3 = .0708
WTM TEMP/DEG K DURING M.B.=299.261111
KGS/SEC IN COND A=1.0867536E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =294.816667
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =607
GC AREA COUNTS, GAS 4 =23230 GAS 5 =41909
GC AREA COUNTS, GAS 6 =10002 GAS 7 =8620

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.026	27	1.56	1	0	27	0
2	.013	28	2.99	2	0	28	0
3	.042	29	32.793	3	0	29	0
4	.099	30	15.805	4	0	30	0
5	.031	31	1.851	5	0	31	0
6	1.146	32	2.793	6	0	32	0
7	.178	33	.843	7	0	33	0
8	0	34	2.23	8	0	34	0
9	.399	35	.086	9	0	35	0
10	.377	36	.229	10	0	36	0
11	.086	37	.351	11	0	37	0
12	0	38	0	12	0	38	0
13	0	39	1.556	13	0	39	0
14	.475	40	.832	14	0	40	0
15	.055	41	1.659	15	0	41	0
16	.04	42	1.059	16	0	42	0
17	.016	43	.41	17	0	43	0
18	.071	44	1.12	18	0	44	0
19	.104	45	.647	19	0	45	0
20	.267	46	1.459	20	0	46	0
21	.25	47	.815	21	0	47	0
22	1.87	48	11.274	22	0	48	0
23	3.023	49	2.157	23	0	49	0
24	.726	50	2.116	24	0	50	0
25	1.378	51	0	25	0	51	0
26	2.698	52	0	26	0	52	0
		53	0			53	0

```
RUN NUMBER  121   MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES
COMPOUND          KG-MOLE/SECOND          KG/S
T-DECALIN      2.68880087E-09          3.7172672E-07
C-DECALIN      4.18794194E-09          5.78982973E-07
TETRALIN      1.01310312E-10          1.33942363E-08
FLUORENE      1.55198039E-09          2.57985701E-07
TOTAL KG-MOLE FED/S =  8.53003351E-09
TOTAL   KGS FED/S =  1.22208963E-06
PUMP RATE/ M3/S  =  1.42143197E-09
TOTAL KG-ATOMS CARBON=   3.23840004E-04
TOTAL KG-ATOMS HYDROGEN=   5.05856787E-04


FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 44.2747351
WHSV (1/S) LIQ FEED BASIS=  3.43203733E-04
VHSV (1/S) =        2.12152329E-04
TOTAL WHSV (1/S) = 5.55325702E-04
MOLAR GAS DENSITY =.269315419  KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC    =4.6723228
SUPERFICIAL GAS VELOCITY/  M/S   =   7.31620543E-03


MATERIAL BALANCE CLOSURE RESULTS
KGS/S,COND A= 1.08667536E-06  KGS/S,COND B= 0
KG-MOLE/S  OF ALL GAS OUT= 3.76801951E-07
H2 FEEDRATE KG-MOLE/S  = 3.77664974E-07
FRACTION OF GAS THAT IS HYDROCARBONS =2.80460311E-03
KG-MOLE/S FREE H2 IN GAS=  3.75745172E-07
H BALANCE CLOSURE = 98.0421602  C BALANCE CLOSURE=94.110986
                    PRODUCT DISTRIBUTION
          WITH FEEDSTOCK                WITHOUT FEEDSTOCK
COMPOUND GROUP CONC./KG-MOLE/M3   COMP. GROUP   MOLE FRAC.
        1       7.60949943E-04        1       .254825845
        2       1.48715624E-04        2       .0498016787
        3       3.4027514E-05         3       .011395086
        4       6.25485191E-04        4       .2094616
        5       0                     5       0
        6       3.2806875E-04         6       .109863201
        7       1.8047909E-03         7       0
        8       8.69841738E-04        8       0
        9       4.85147895E-05        9       0
        10      3.01921331E-04        10      .10110699
        11      3.67526068E-04        11      .123076612
        12      3.30141901E-04        12      .110557455
        13      5.16035415E-04        13      0
        14      8.93205261E-05        14      .029911532
        H2      .263090079
KG-MOLE FLUORENE/S  IN PRODUCT =  7.37001625E-10
FLUORENE CONVERSION =  52.512182  %
T-DECALIN CONVERSION=  4.13563734  %
C-DECALIN CONVERSION=  70.3360809  %
```

RUN NUMBER =122 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN122PR
PUMP TEMP/ DEG K =394.261111
INITIAL TIME OF M. B./S =9351 FINAL TIME=13030.8
INITIAL PUMP VOL/M3= 6.079E-05 FINAL VOL/M3= 7.127E-05
WT % OF TRANS-DECALIN =30.921
CIS-DECALIN = 48.593
TETRALIN = 1.139
FLUORENE = 19.347
BAROMETRIC PRESSURE/ BARS =1.0181702
P CORRECTION/ BARS = 4.09706E-03
H20 VAPOR PRESS/ BARS = .0431715
WTM SEC/REV AVERAGE=77.4 WTM TEMP/K=301.205556
KGMS OF CATALYST =3.0355E-03 VOLUME/M3=5.5E-06
REACTOR PRESS/BARS=35.8330392 REACTOR TEMP/K=660.372223
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=303.427778
KGS/SEC IN COND A=2.42049918E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =298.705556
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =1743
GC AREA COUNTS, GAS 4 =27181 GAS 5 =49192
GC AREA COUNTS, GAS 6 =11793 GAS 7 =6922

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.078	27	2.475	1	0	27	0
2	.036	28	4.37	2	0	28	0
3	.077	29	34.787	3	0	29	0
4	.189	30	9.278	4	0	30	0
5	.067	31	1.955	5	0	31	0
6	2.198	32	2.948	6	0	32	0
7	.304	33	1.352	7	0	33	0
8	0	34	1.966	8	0	34	0
9	.769	35	.043	9	0	35	0
10	.721	36	.1	10	0	36	0
11	.157	37	.092	11	0	37	0
12	.03	38	.21	12	0	38	0
13	0	39	.486	13	0	39	0
14	.655	40	.202	14	0	40	0
15	.114	41	.381	15	0	41	0
16	.07	42	.417	16	0	42	0
17	.074	43	.078	17	0	43	0
18	.132	44	.446	18	0	44	0
19	.156	45	.139	19	0	45	0
20	.314	46	.596	20	0	46	0
21	.378	47	.249	21	0	47	0
22	2.693	48	9.048	22	0	48	0
23	8.052	49	2.126	23	0	49	0
24	0	50	2.031	24	0	50	0
25	2.327	51	0	25	0	51	0
26	4.64	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 122 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.45559778E-09	7.54236393E-07
C-DECALIN	8.57358633E-09	1.18529831E-06
TETRALIN	2.10142247E-10	2.77829065E-08
FLUORENE	2.83895285E-09	4.71919132E-07

TOTAL KG-MOLE FED/S = 1.70782792E-08
TOTAL KGS FED/S = 2.43923674E-06
PUMP RATE/ M3/S = 2.84800365E-09
TOTAL KG-ATOMS CARBON= 6.45473578E-04
TOTAL KG-ATOMS HYDROGEN= 1.02036341E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.516915
WHSV (1/S) LIQ FEED BASIS= 8.03563574E-04
VHSV (1/S) = 5.17814704E-04
TOTAL WHSV (1/S) = 1.27072338E-03
MOLAR GAS DENSITY =.652504469 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.94246725
SUPERFICIAL GAS VELOCITY/ M/S = 5.67757419E-03

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.42032492E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.10618883E-07
H2 FEEDRATE KG-MOLE/S = 7.09037466E-07
FRACTION OF GAS THAT IS HYDROCARBONS =3.25612682E-03
KG-MOLE/S FREE H2 IN GAS= 7.08305018E-07
H BALANCE CLOSURE = 100.461965 C BALANCE CLOSURE=104.469019

PRODUCT DISTRIBUTION

WITH FEEDSTOCK		WITHOUT FEEDSTOCK	
COMPOUND GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
1	2.20216623E-03	1	.222795504
2	8.15297274E-04	2	.0824844938
3	1.95467414E-04	3	.0197756465
4	2.52202445E-03	4	.2551559
5	0	5	0
6	2.01524695E-03	6	.20388468
7	5.45389727E-03	7	0
8	1.45460255E-03	8	0
9	2.21649881E-04	9	0
10	8.69777421E-04	10	.0879963083
11	5.30008514E-04	11	.053621526
12	4.9003593E-04	12	.0495774571
13	1.17977259E-03	13	0
14	2.44224802E-04	14	.0247084834
H2	.634310298		

KG-MOLE FLUORENE/S IN PRODUCT = 1.31739757E-09
FLUORENE CONVERSION = 53.5956516 %
T-DECALIN CONVERSION= -11.6305759 %
C-DECALIN CONVERSION= 81.0547485 %

RUN NUMBER =123 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN123PR
PUMP TEMP/ DEG K =395.094445
INITIAL TIME OF M. B./S =8807.4 FINAL TIME=12541.8
INITIAL PUMP VOL/M3= 9.552E-05 FINAL VOL/M3= 1.0613E-04
WT % OF TRANS-DECALIN =30.921
CIS-DECALIN = 48.593
TETRALIN = 1.139
FLUORENE = 19.347
BAROMETRIC PRESSURE/ BARS =1.0120754
P CORRECTION/ BARS = 4.60496E-03
H20 VAPOR PRESS/ BARS = .04005638
WTM SEC/REV AVERAGE=78 WTM TEMP/K=301.622223
KGMS OF CATALYST =4.1292E-03 VOLUME/M3=7.65E-06
REACTOR PRESS/BARS=25.1457892 REACTOR TEMP/K=660.705556
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=302.177778
KGS/SEC IN COND A=2.2732374E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =298.15
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =2992
GC AREA COUNTS, GAS 4 =33591 GAS 5 =60170
GC AREA COUNTS, GAS 6 =13504 GAS 7 =8417

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	.094	27	2.886	1	0	27	0
2	.052	28	4.153	2	0	28	0
3	.152	29	34.322	3	0	29	0
4	.277	30	6.967	4	0	30	0
5	.098	31	2.541	5	0	31	0
6	3.138	32	3.84	6	0	32	0
7	.446	33	1.331	7	0	33	0
8	.246	34	2.592	8	0	34	0
9	1.091	35	.045	9	0	35	0
10	.947	36	.133	10	0	36	0
11	.206	37	.129	11	0	37	0
12	.039	38	.25	12	0	38	0
13	0	39	.663	13	0	39	0
14	1.057	40	.266	14	0	40	0
15	.132	41	.372	15	0	41	0
16	.08	42	.374	16	0	42	0
17	.067	43	.077	17	0	43	0
18	.132	44	.424	18	0	44	0
19	.198	45	.128	19	0	45	0
20	.447	46	.619	20	0	46	0
21	.462	47	.227	21	0	47	0
22	2.219	48	7.541	22	0	48	0
23	5.785	49	2.099	23	0	49	0
24	1.455	50	2.312	24	0	50	0
25	2.271	51	0	25	0	51	0
26	4.62	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 123 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.43793815E-09	7.5179495E-07
C-DECALIN	8.54583385E-09	1.18146153E-06
TETRALIN	2.09462022E-10	2.7692974E-08
FLUORENE	2.82976323E-09	4.70391542E-07

TOTAL KG-MOLE FED/S = 1.70229973E-08
TOTAL KGS FED/S = 2.431341E-06
PUMP RATE/ M3/S = 2.84117525E-09
TOTAL KG-ATOMS CARBON= 6.43384197E-04
TOTAL KG-ATOMS HYDROGEN= 1.01706053E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 41.1260198
WHSV (1/S) LIQ FEED BASIS= 5.88811767E-04
VHSV (1/S) = 3.71392488E-04
TOTAL WHSV (1/S) = 9.27900463E-04
MOLAR GAS DENSITY =.457664721 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =4.88231605
SUPERFICIAL GAS VELOCITY/ M/S = 7.9942822E-03

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.27307374E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.00598192E-07
H2 FEEDRATE KG-MOLE/S = 7.00088122E-07
FRACTION OF GAS THAT IS HYDROCARBONS =4.00645603E-03
KG-MOLE/S FREE H2 IN GAS= 6.97791276E-07
H BALANCE CLOSURE = 99.5536131 C BALANCE CLOSURE=99.7538477

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	1.91957609E-03	1	.251007068
	2	7.64204737E-04	2	.0999287243
	3	2.07831812E-04	3	.0271764448
	4	1.90091197E-03	4	.248566515
	5	0	5	0
	6	1.14701212E-03	6	.149985276
	7	3.59785688E-03	7	0
	8	7.30326581E-04	8	0
	9	1.45898285E-04	9	0
	10	7.54666361E-04	10	.09868147
	11	4.46548278E-04	11	.05839142
	12	3.20859812E-04	12	.0419561802
	13	6.57439771E-04	13	0
	14	1.85886989E-04	14	.0243069021
	H2	.444885702		

KG-MOLE FLUORENE/S IN PRODUCT = 1.03117663E-09
FLUORENE CONVERSION = 63.5596147 %
T-DECALIN CONVERSION= -3.77355804 %
C-DECALIN CONVERSION= 86.5958355 %

RUN NUMBER =124 INPUT DATA FOR M.B.
DATA IS FILED UNDER RUN124PR
PUMP TEMP/ DEG K =395.927778
INITIAL TIME OF M. B./S =9661.8 FINAL TIME=13380.6
INITIAL PUMP VOL/M3= 1.3195E-04 FINAL VOL/M3= 1.4251E-04
WT % OF TRANS-DECALIN =30.921
CIS-DECALIN = 48.593
TETRALIN = 1.139
FLUORENE = 19.347
BAROMETRIC PRESSURE/ BARS =1.0117368
P CORRECTION/ BARS = 4.4018E-03
H20 VAPOR PRESS/ BARS = .04171552
WTM SEC/REV AVERAGE=78.18 WTM TEMP/K=301.9
KGMS OF CATALYST =.0136094 VOLUME/M3=2.45E-05
REACTOR PRESS/BARS=8.1840892 REACTOR TEMP/K=660.872223
INITIAL WTM M3 = 0 FINAL M3 = .067968
WTM TEMP/DEG K DURING M.B.=302.872223
KGS/SEC IN COND A=2.114058E-06 KGS/SEC IN B = 0
ROOM TEMP/DEG K =298.15
GAS SAMPLE INJ VOLUME/M3 =1E-06
GC AREA COUNTS, GAS 2 =0 GAS 3 =1835
GC AREA COUNTS, GAS 4 =41103 GAS 5 =77065
GC AREA COUNTS, GAS 6 =17503 GAS 7 =20257

WEIGHT % PRODUCT FROM G.C. ANALYSIS

CONDENSER A				CONDENSER B			
COMP#	WT%	COMP#	WT%	COMP#	WT%	COMP#	WT%
1	7E-03	27	2.834	1	0	27	0
2	.033	28	3.156	2	0	28	0
3	.064	29	33.292	3	0	29	0
4	.201	30	6.108	4	0	30	0
5	.073	31	4.059	5	0	31	0
6	2.606	32	7.327	6	0	32	0
7	.59	33	0	7	0	33	0
8	0	34	4.832	8	0	34	0
9	.895	35	.041	9	0	35	0
10	.819	36	.164	10	0	36	0
11	.178	37	.3	11	0	37	0
12	0	38	.385	12	0	38	0
13	0	39	1.481	13	0	39	0
14	1.219	40	.615	14	0	40	0
15	.113	41	.481	15	0	41	0
16	.065	42	.474	16	0	42	0
17	.054	43	.252	17	0	43	0
18	.101	44	.583	18	0	44	0
19	.266	45	.124	19	0	45	0
20	.818	46	.579	20	0	46	0
21	.466	47	.372	21	0	47	0
22	1.873	48	6.998	22	0	48	0
23	3.873	49	2.236	23	0	49	0
24	1.509	50	2.887	24	0	50	0
25	1.458	51	0	25	0	51	0
26	3.137	52	0	26	0	52	0
		53	0			53	0

RUN NUMBER 124 MATERIAL BALANCE OUTPUT
FEEDSTOCK COMPOSITION AND FLOWRATES

COMPOUND	KG-MOLE/SECOND	KG/S
T-DECALIN	5.43042914E-09	7.50756828E-07
C-DECALIN	8.53403328E-09	1.1798301E-06
TETRALIN	2.09172785E-10	2.76547339E-08
FLUORENE	2.82585574E-09	4.69741999E-07

TOTAL KG-MOLE FED/S = 1.69994909E-08
TOTAL KGS FED/S = 2.42798366E-06
PUMP RATE/ M3/S = 2.8396484E-09
TOTAL KG-ATOMS CARBON= 6.42495776E-04
TOTAL KG-ATOMS HYDROGEN= 1.01565611E-03

FEED/CATALYST RATIOS
H2/HYDROCARBON RATIO= 40.9741373
WHSV (1/S) LIQ FEED BASIS= 1.78403474E-04
VHSV (1/S) = 1.15903089E-04
TOTAL WHSV (1/S) = 2.80764181E-04
MOLAR GAS DENSITY =.14891995 KG-MOLE/M3
SPACE TIME AT RXN CONDITIONS/SEC =5.1133409
SUPERFICIAL GAS VELOCITY/ M/S = .0244458569

MATERIAL BALANCE CLOSURE RESULTS
KGS/S IN COND A= 2.1139058E-06 KGS/S IN COND B= 0
KG-MOLE/S OF ALL GAS OUT= 7.00622904E-07
H2 FEEDRATE KG-MOLE/S = 6.96539475E-07
FRACTION OF GAS THAT IS HYDROCARBONS =5.2172424E-03
KG-MOLE/S FREE H2 IN GAS= 6.96967584E-07
H BALANCE CLOSURE = 98.8615422 C BALANCE CLOSURE=95.65

PRODUCT DISTRIBUTION

WITH FEEDSTOCK			WITHOUT FEEDSTOCK	
COMPOUND	GROUP	CONC./KG-MOLE/M3	COMP. GROUP	MOLE FRAC.
	1	7.80608592E-04	1	.297311176
	2	1.90555512E-04	2	.0725770688
	3	4.31845212E-05	3	.0164477318
	4	5.09111961E-04	4	.193905983
	5	0	5	0
	6	2.59480381E-04	6	.0988285524
	7	1.05800623E-03	7	0
	8	1.94109757E-04	8	0
	9	0	9	0
	10	4.05117188E-04	10	.154297389
	11	2.57823442E-04	11	.0981974725
	12	1.09309693E-04	12	.0416328924
	13	1.84960082E-04	13	0
	14	7.03695847E-05	14	.0268017342
	H2	.144857314		

KG-MOLE FLUORENE/S IN PRODUCT = 8.89918353E-10
FLUORENE CONVERSION = 68.5080048 %
T-DECALIN CONVERSION= 6.25972454 %
C-DECALIN CONVERSION= 89.0562746 %

APPENDIX 4

Computer Program Listings

Program Usage Summary

The computer program code listings which follow the summary below were used to perform the material balance calculations and estimate the rate constants and activation energies of the kinetic models presented in the text. The BASIC codes were implemented on an Apple IIe personal computer and the FORTRAN codes were run on the IBM 3081 mainframe at Louisiana State University. The codes are self supporting except for the LSODE routine, which is on direct access disk at the L.S.U. S.N.C.C.

BASIC listings:

MATBALSICONC is the main program for material balance calculations. After supplying the data set name for the experimental run of interest, it performs the calculations described in Appendix 2 and prints the material balance outputs as those listed in Appendix 3 for each run. One call is made to MATBALDATA for molecular weights and carbon and hydrogen numbers for the feed and product compounds. Output is in S.I. notation.

MATBALDATA data set contains the molecular weights and carbon and hydrogen numbers of the compounds.

LOADER and READER are utility programs for input and output of MATBALDATA.

DATASTORE is an interactive program to store the experimental run and analytical data on disk under a user supplied data set name. Data input must correspond to the units requested from the program.

DATAPRTSI provides the output from the dataset stored by DATASTORE. This output is listed in Appendix 3 as input data for the material

balance. The routine converts the raw experimental data to S.I. notation.

HJB.KINETIC.FIT calculates the experimental rate constants for the kinetic model of interest. Concentration vs. space time data are called from a data set (ex: KINDAT730-2) and using the H.J.B. method, integration of the concentration terms is performed by trapezoid rule wherein the resulting matrices are solved by a Gauss-Jordon routine converted to BASIC from the FORTRAN code developed in Carnahan et al. (1969) using the term scaled pivoting method. The user supplied matrix terms from line 2000 to 2600 define the concentration terms of the kinetic model of interest.

KINDAT.10.2 is used as a utility to store and recall the concentration vs. space time data of the data set called by HJB.KINETIC.FIT.

KINDAT730-2 data set contains the concentration vs. space time data which is called by the HJB.KINETIC.FIT routine.

FORTRAN listings:

FIT730 program is a pattern search routine with an acceleration step that was used to estimate rate constants with the constraint that all rate constants be positive. The routine is a copy of Moore, Smith, and Murrill's (1969) program obtained from the Chemical Engineering Department at L.S.U. with modifications to contain the integration of the H.J.B. method. Optimization is based on minimizing the sum of squares of the weighted deviations of the concentration terms. In addition to the data required by the pattern search routine itself, the

user must also supply the matrix of concentration terms for the kinetic model.

ACTIV is the same pattern search routine as FIT730 except that in this case the activation energies are estimated. Concentration vs. space time, base rate constants, and concentration vs. temperature data are required for the optimization along with the matrix of concentration terms. The minimum of the sum of squares of the weighted deviations of concentration is optimized over the temperature range of the data. The activation energies are constrained to be positive by subroutine BOUNDS.

KINT730 is supported by the called routine LSODE employing the Gear-Hindmarsh integration method (Hindmarsh, 1980). This routine was used to solve the differential equations of the kinetic model once the rate constants had been determined by the H.J.B. method. The program requires the initial concentrations and the equations of the model (YDOT) to be solved. Application of this program is straightforward and is discussed in detail in Manual II of the Computer Aids for Engineering Series by the L.S.U. Design Group of the Chemical Engineering Department at Louisiana State University.

PROGRAM MATBALSICONC

```
10  DIM A(138)
20  INPUT "RUN FILE NAME ?";R$
30  PRINT  CHR$ (4);"OPEN"R$",L10"
40  FOR I = 1 TO 138
50  PRINT  CHR$ (4);"READ"R$",R";I
60  INPUT A(I)
70  NEXT I
80  PRINT  CHR$ (4);"CLOSE"R$
90  REM  ***********CALC DENSITY OF FEEDSTOCKS AT PUMP TEMP*
***********
100 R1 = .8699
110 R2 = .8965
120 R3 = .9702
130 R4 = 1.2030
140 T1 = 719.4
150 T2 = 691.16
160 T3 = 681.16
170 T4 = 607.86
180 JUN = A(1)
190 T7 = A(2)
200 RT = 293.16
210 TPK = ((T7 + 460) / 1.8)
220 D1 = R1 * (((T1 - TPK) / (T1 - RT)) ^ .29)
230 D2 = R2 * (((T2 - TPK) / (T2 - RT)) ^ .29)
240 D3 = R3 * (((T3 - TPK) / (T3 - RT)) ^ .29)
250 D4 = R4 * (((T4 - TPK) / (T4 - RT)) ^ .29)
260  REM   ***************CALC G-MOLES,GRAMS, G-ATOMS OF C A
ND H IN FS**
270 T5 = A(3)
280 T6 = A(4)
290 B1 = A(5)
300 B2 = A(6)
310 TI = T6 - T5
320 BT = B2 - B1
330 FR = (BT / TI) * 60
340 WA = A(7)
350 WB = A(8)
360 WC = A(9)
```

```
370 WD = A(10)
380 A = 138.25
390 B = 138.25
400 C = 132.21
410 D = 166.23
420  REM  G ATOMS OF CARBON
430 DA = 10
440 DB = 10
450 DC = 10
460 DD = 13
470  REM  G ATOMS OF HYDROGEN
480 EA = 18
490 EB = 18
500 EC = 12
510 ED = 10
520  REM  CONVERT WT% TO VOL%
530 NA = WA / D1
540 NB = WB / D2
550 NC = WC / D3
560 ND = WD / D4
570 NT = NA + NB + NC + ND
580  REM  CALC CC OF EACH COMPOUND
590 VA = NA / NT
600 VB = NB / NT
610 VC = NC / NT
620 VD = ND / NT
630 CA = VA * FR
640 CB = VB * FR
650 CC = VC * FR
660 CD = VD * FR
670  REM  CALC THE G MOLES OF EACH AND TOTAL
680 MA = CA * D1 / A
690 MB = CB * D2 / B
700 MC = CC * D3 / C
710 MD = CD * D4 / D
720 TM = MA + MB + MC + MD
730  REM  CALC THE GRAMS OF EACH AND TOTAL
740 QA = CA * D1
750 QB = CB * D2
760 QC = CC * D3
770 QD = CD * D4
780 WT = QA + QB + QC + QD
790  PRINT  CHR$ (4);"PR#1"
800  PRINT  CHR$ (9);"80N"
810  PRINT  CHR$ (9);"10L"
820  PRINT "RUN NUMBER  ";JUN;"   MATERIAL BALANCE OUTPUT"
830  PRINT "FEEDSTOCK COMPOSITION AND FLOWRATES"
840  PRINT "COMPOUND          KG-MOLE/SECOND          KG/S "
850  PRINT "T-DECALIN"; SPC( 5);MA * 2.7778 * 10 ^  - 7; SPC(
12);QA * 2.7778 * 10 ^  - 7
860  PRINT "C-DECALIN"; SPC( 5);MB * 2.7778 * 10 ^  - 7; SPC(
12);QB * 2.7778 * 10 ^  - 7
870  PRINT "TETRALIN"; SPC( 5);MC * 2.7778 * 10 ^  - 7; SPC(
12);QC * 2.7778 * 10 ^  - 7
```

```
880  PRINT "FLUORENE"; SPC( 5);MD * 2.7778 * 10 ^  - 7; SPC(
12);QD * 2.7778 * 10 ^  - 7
890  PRINT "TOTAL KG-MOLE FED/S ="; SPC( 2);TM * 2.7778 * 10
 ^  - 7
900  PRINT "TOTAL   KGS FED/S ="; SPC( 2);WT * 2.7778 * 10 ^
 - 7
910  PRINT "PUMP RATE/ M3/S  =  ";FR * 2.7778 * 10 ^  - 10
920  REM  CALC THE # OF CARBON AND HYDROGEN ATOMS TOTAL
930 HA = MA * EA + MB * EB + MC * EC + MD * ED
940 CR = MA * DA + MB * DB + MC * DC + MD * DD
950 CFS = CR
960  PRINT "TOTAL KG-ATOMS CARBON= "; SPC( 2);CR / 1000
970  PRINT "TOTAL KG-ATOMS HYDROGEN= "; SPC( 2);HA / 1000
980  PRINT  CHR$ (4);"PR#0"
990  PRINT  CHR$ (4);"PR#3"
1000  REM   **************CALC GAS FLOWRATES,SPACE VELS.,FEED
 RATIOS***
1010  REM  THE FOLLOWING STATEMENTS OF INPUT FEED IN THE RUN
 CONDITIONS
1020 BP = A(11)
1030 CR = A(12)
1040 VP = A(13)
1050 MIN = A(14)
1060 TWTM = A(15)
1070 HCT = TM
1080 WCT = A(16)
1090 VCT = A(17)
1100 LV = FR
1110 LW = WT
1120 P = A(18)
1130 T = A(19)
1140  REM  CALC THE MOLES PER HOUR OF GAS AT THE WTM
1150 N = (14.7 * (BP - CR - VP) * 0.05 * 60 * 453.6) / (29.9
2 * MIN * 10.732 * (460 + TWTM))
1160 HHCR = N / HCT
1165 MGD = ((P + 14.7) * 453.6) / (10.732 * (T + 460) * 2831
2.6)
1170  IF WCT = 0 THEN  GOTO 1260
1180  IF VCT = 0 THEN  GOTO 1260
1190 WHRW = LW / WCT
1200 VHRV = LV / VCT
1220 SRT = (MGD * VCT * 3600) / (N + HCT)
1230 SGV = VCT / (1.96 * SRT)
1240 ZTW = ((N * 2) + LW) / WCT
1250  GOTO 1300
1260 WHRW = 0
1270 VHRV = 0
1280 SGV = 0
1290 ZTW = 0
1300  PRINT  CHR$ (4);"PR#1"
1310  PRINT  CHR$ (9);"80N"
1320  PRINT  CHR$ (9);"10L"
1330  PRINT "FEED/CATALYST RATIOS"
1340  PRINT "H2/HYDROCARBON RATIO= ";HHCR
```

```
1350  PRINT "WHSV (1/S) LIQ FEED BASIS=  ";WHRW / 3600
1355  PRINT "VHSV (1/S) =        ";VHRV / 3600
1360  PRINT "TOTAL WHSV (1/S) = ";ZTW / 3600
1370  PRINT "MOLAR GAS DENSITY =";MGD * 1000;"  KG-MOLE/M3"
1380  PRINT "SPACE TIME AT RXN CONDITIONS/SEC    =";SRT
1390  PRINT "SUPERFICIAL GAS VELOCITY/  M/S   ="; SPC( 3);SG
V / 100
1400  PRINT  CHR$ (4);"PR#0"
1410  PRINT  CHR$ (4);"PR#3"
1420  REM  NAME GASRATE
1430  REM  PROGRAM TO CALC GAS OUTPUT IN MOLES/HR DURING MAT
L BAL
1440  REM  THE FOLLOWING STATEMENTS OF INPUT FEED IN THE RUN
 CONDITIONS
1450 V1 = A(20)
1460 V2 = A(21)
1470 TWTM = A(22)
1480 MIN = ((T6 - T5) / (V2 - V1)) * 0.05
1490  REM  CALC THE MOLES PER HOUR OF GAS AT THE WTM
1500 NM = (14.7 * (BP - CR - VP) * 0.05 * 60 * 453.6) / (29.
92 * MIN * 10.732 * (460 + TWTM))
1510  REM   ***********MATERIAL BALANCE CALCULATIONS********
***
1520 T = 106
1530  DIM MW(T),AC(T),AH(T),WT(T),GM(T),C(T),H(T),HCT(14),LA
ST(14),LLAST(14),CN(7),GS(7),GA(7)
1540 AWT = A(23)
1550 BWT = A(24)
1560 NT = NM
1570 H2R = N
1580 HF = HA
1590 RT = A(25)
1600 VO = A(26)
1610 TT = (((BP - CR) / 29.92) * (VO / 1000)) / (0.08206 * (
(RT + 460) / 1.8))
1620 CN(5) = TT * 0.010685 / (333643 * VO)
1630 CN(6) = CN(5)
1640 CN(2) = CN(6) * 2.439 / 1.149
1650 CN(3) = CN(6) * 1.724 / 1.149
1660 CN(4) = CN(6) * 1.3699 / 1.149
1670 CN(7) = CN(6) * 0.94065 / 1.149
1680  FOR I = 2 TO 7
1690 GA(I) = A(I + 25)
1700 GS(I) = GA(I) * CN(I)
1710  NEXT I
1720 GS(1) = GS(2) + GS(3) + GS(4) + GS(5) + GS(6) + GS(7)
1730  IF GS(1) = 0 THEN  GOTO 1830
1740  REM  4.1031*10^-5 IS MOLS/CC IN SYRINGE AT ROOM TEMP A
ND PRESS.
1750 Y = GS(1) / TT
1760 G2 = (GS(2) / GS(1)) * 100
1770 G3 = (GS(3) / GS(1)) * 100
1780 G4 = (GS(4) / GS(1)) * 100
1790 G5 = (GS(5) / GS(1)) * 100
```

```
1800 G6 = (GS(6) / GS(1)) * 100
1810 G7 = (GS(7) / GS(1)) * 100
1820  GOTO 1900
1830 Y = 0
1840 G2 = 0
1850 G3 = 0
1860 G4 = 0
1870 G5 = 0
1880 G6 = 0
1890 G7 = 0
1900  PRINT  CHR$ (4);"OPEN MATLBALDATA"
1910  PRINT  CHR$ (4);"READ MATLBALDATA"
1920  FOR I = 1 TO T
1930  INPUT MW(I)
1940  NEXT I
1950  FOR I = 1 TO T
1960  INPUT AC(I)
1970  NEXT I
1980  FOR I = 1 TO T
1990  INPUT AH(I)
2000  NEXT I
2010  PRINT  CHR$ (4);"CLOSE MATLBALDATA"
2020  FOR I = 1 TO T
2030 WT(I) = A(I + 32)
2040  NEXT I
2050  REM  CALC THE GRAM MOLES OF EACH
2060  FOR I = 1 TO T
2070  IF I > 53 THEN  GOTO 2100
2080 GM(I) = ((WT(I) / 100) * AWT) / MW(I)
2090  GOTO 2110
2100 GM(I) = ((WT(I) / 100) * BWT) / MW(I)
2110 C(I) = AC(I) * GM(I)
2120 H(I) = AH(I) * GM(I)
2130  NEXT I
2140  REM  INITIALIZE ALL TOTALS TO ZERO
2150 C = 0
2160 H = 0
2170 GM = 0
2180  REM  CALC TOTAL G ATOMS OF C AND H IN CONDENSERS
2190  FOR I = 1 TO T
2200 C = C + C(I)
2210 H = H + H(I)
2220 GM = GM + GM(I)
2230  NEXT I
2240  REM  CALCS FOR GAS BALANCE
2250  REM  CALC THE G ATOMS OF H IN GAS
2260 HTI = HF + 2 * H2R
2270 HGAS = HTI - H
2280  REM   CALC G MOLES OF EACH ONE IN GAS AND G ATOMS C AN
D H AND SUM
2290 GH2 = (1 - Y) * NT
2300 M2GAS = Y * G2 * NT / 100
2310 M3GAS = Y * G3 * NT / 100
2320 M4GAS = Y * G4 * NT / 100
```

```
2330 M5GAS = Y * G5 * NT / 100
2340 M6GAS = Y * G6 * NT / 100
2350 M7GAS = Y * G7 * NT / 100
2360 SUMGAS = M2GAS + M3GAS + M4GAS + M5GAS + M6GAS + M7GAS
2370 CGAS = M2GAS * 1 + M3GAS * 2 + M4GAS * 3 + M5GAS * 4 +
M6GAS * 4 + M7GAS * 5
2380  REM  HALL=H IN HYDROCARBONS IN GAS
2390 HALL = M2GAS * 4 + M3GAS * 6 + M4GAS * 8 + M5GAS * 10 +
M6GAS * 10 + M7GAS * 12
2400 COUT = CGAS + C
2410 CBAL = (COUT / CFS) * 100
2420 HBAL = ((H + HALL + (2 * GH2)) / (H2R * 2 + HF)) * 100
2430  REM  CALC THE TOTAL G MOLES OF EACH FOR PRODUCT GROUPI
NG
2440  REM  HCT(1)=ALKANES, 2=CPT, 3=CHX, 4=BZ, 5=ALKYLBZ, 6=
DMOHP, 7=TDEC, 8=CDEC,9=TET, 10=INDANS, 11=NAPHTH, 12=BIPH,
13=FLUORENE, 14=METHYLFLUORENE
2450 HCT(1) = SUMGAS + GM(1) + GM(2) + GM(3) + GM(4) + GM(5)
 + GM(54) + GM(55) + GM(56) + GM(57) + GM(58)
2460 HCT(2) = GM(6) + GM(59) + GM(9) + GM(62) + GM(11) + GM(
64) + GM(12) + GM(65) + GM(13) + GM(66) + GM(16) + GM(69) +
GM(18) + GM(71)
2470 HCT(3) = GM(8) + GM(61) + GM(10) + GM(63) + GM(15) + GM
(68) + GM(17) + GM(70)
2480 HCT(4) = GM(7) + GM(60) + GM(14) + GM(67) + GM(19) + GM
(20) + GM(21) + GM(72) + GM(73) + GM(74) + GM(22) + GM(75) +
GM(24) + GM(77) + GM(26) + GM(79) + GM(28) + GM(81)
2490 HCT(5) = GM(51) + GM(52) + GM(53) + GM(104) + GM(105) +
GM(106)
2500 HCT(6) = GM(23) + GM(25) + GM(27) + GM(76) + GM(78) + G
M(80)
2510 HCT(7) = GM(29) + GM(82)
2520 HCT(8) = GM(30) + GM(83)
2530 HCT(9) = GM(33) + GM(86)
2540 HCT(10) = GM(31) + GM(84) + GM(32) + GM(85) + GM(35) +
GM(88) + GM(36) + GM(89) + GM(37) + GM(90) + GM(38) + GM(91)

2550 HCT(11) = GM(34) + GM(87) + GM(39) + GM(92) + GM(40) +
GM(93) + GM(43) + GM(96) + GM(44) + GM(97) + GM(45) + GM(98)

2560 HCT(12) = GM(41) + GM(94) + GM(42) + GM(95) + GM(46) +
GM(99) + GM(47) + GM(100) + GM(49) + GM(102)
2570 HCT(13) = GM(48) + GM(101)
2580 FL = HCT(13)
2585 CX = 0
2590 CY = 0
2600 CZ = 0
2610  IF MA = 0 THEN  GOTO 2630
2620 CY = ((MA - HCT(7)) / MA) * 100
2630  IF MB = 0 THEN  GOTO 2642
2640 CZ = ((MB - HCT(8)) / MB) * 100
2642  IF MA + MB = 0 THEN  GOTO 2650
2645 CX = (((MA + MB) - (HCT(7) + HCT(8))) / (MA + MB)) * 10
0
```

```
2650 CN = 0
2660  IF FL = 0 THEN  GOTO 2690
2670  IF MD = 0 THEN  GOTO 2690
2680 CN = ((MD - FL) / MD) * 100
2690 HCT(14) = GM(50) + GM(103)
2700  REM  CALC MOLE FRACTION OF PRODUCTS INCLUDING FEEDSTOC
K
2710 ZHCT = 0
2720  FOR I = 1 TO 14
2730 ZHCT = ZHCT + HCT(I)
2740  NEXT I
2750  FOR I = 1 TO 14
2760 LAST(I) = (HCT(I) / (ZHCT + GH2)) * (MGD * 1000)
2770  NEXT I
2780  REM  REMOVE FEEDSTOCKS FROM CALC
2790  IF A(7) = 0 THEN  GOTO 2810
2800 HCT(7) = 0
2810  IF A(8) = 0 THEN  GOTO 2830
2820 HCT(8) = 0
2830  IF A(9) = 0 THEN  GOTO 2850
2840 HCT(9) = 0
2850  IF A(10) = 0 THEN  GOTO 2880
2860  REM  CALC MOLE FRACTIONS OF PRODUCTS W/O FEEDSTOCK
2870 HCT(13) = 0
2880 YTHC = 0
2890  FOR I = 1 TO 14
2900 YTHC = YTHC + HCT(I)
2910  NEXT I
2920  FOR I = 1 TO 14
2930 LLAST(I) = HCT(I) / YTHC
2940  NEXT I
2950 D$ =  CHR$ (13) +  CHR$ (4)
2960  PRINT D$;"PR#1"
2970  PRINT  CHR$ (9);"80N"
2980  PRINT  CHR$ (9);"10L"
2990  PRINT "MATERIAL BALANCE CLOSURE RESULTS"
3000  PRINT "  KGS/S  IN COND A= ";AWT * 2.7778 * 10 ^  - 7;
"   KGS/S IN COND B= ";BWT * 2.7778 * 10 ^  - 7
3010  PRINT "KG-MOLE/S  OF ALL GAS OUT= ";NT * 2.7778 * 10 ^
 - 7
3020  PRINT "H2 FEEDRATE KG-MOLE/S  = ";H2R * 2.7778 * 10 ^
 - 7
3030  PRINT "FRACTION OF GAS THAT IS HYDROCARBONS =";Y
3040  PRINT "KG-MOLE/S FREE H2 IN GAS=  ";GH2 * 2.7778 * 10 ^
 - 7
3050  PRINT "H BALANCE CLOSURE = ";HBAL;"  C BALANCE CLOSURE
=";CBAL
3060  PRINT  SPC( 22);"PRODUCT DISTRIBUTION"
3070  PRINT  SPC( 10);"WITH FEEDSTOCK"; SPC( 15);"WITHOUT FE
EDSTOCK"
3080  PRINT "COMPOUND GROUP CONC./KG-MOLE/M3   COMPOUND GROU
P   MOLE FRACTION"
3090  FOR I = 1 TO 14
3100  HTAB 20: PRINT I;
```

```
3110  HTAB 28: PRINT LAST(I);
3120  POKE 36,53: PRINT I;
3130  POKE 36,61: PRINT LLAST(I)
3140  NEXT I
3145  HTAB 20: PRINT "H2";
3146  HTAB 28: PRINT (GH2 / (ZHCT + GH2)) * MGD * 1000
3150  PRINT "KG-MOLE FLUORENE/S  IN PRODUCT =  ";FL * 2.7778
 * 10 ^  - 7
3160  PRINT "FLUORENE CONVERSION =  ";CN;"  %"
3170  PRINT "T-DECALIN CONVERSION=  ";CY;"  %"
3180  PRINT "C-DECALIN CONVERSION=  ";CZ;"  %"
3185  PRINT "TOTAL DEC CONVERSION=  ";CX;"  %"
3190  PRINT  CHR$ (4);"PR#0"
3200  PRINT  CHR$ (4);"PR#3"
```

DATASET MATBALDATA

58.13	4	10
58.13	4	10
72.15	5	12
86.18	6	14
86.18	6	14
84.16	6	12
78.12	6	6
84.16	6	12
98.19	7	14
98.19	7	14
98.19	7	14
112.22	8	16
112.22	8	16
92.15	7	8
112.22	8	16
112.22	8	16
112.22	8	16
112.22	8	16
106.17	8	10
106.17	8	10
106.17	8	10
120.19	9	12
138.25	10	18
120.19	9	12
138.25	10	18
120.19	9	12
138.25	10	18
138.25	10	18
132.21	10	12
132.21	10	12
132.21	10	12
128.19	10	8
146.21	11	14
146.21	11	14
146.21	11	14
146.21	11	14
142.2	11	10
142.2	11	10
154.21	12	10
168.24	13	12
146.23	12	12
156.23	12	12
156.23	12	12
168.24	13	12
168.24	13	12
166.23	13	10
168.24	13	12
180.25	14	12
118	9	10
134	10	14
132	10	12
58.13	4	10
58.13	4	10
72.15	5	12
86.18	6	14
86.18	6	14
84.16	6	12
78.12	6	6
84.16	6	12
98.19	7	14
98.19	7	14
98.19	7	14
112.22	8	16
112.22	8	16
92.15	7	8
112.22	8	16
112.22	8	16
112.22	8	16
112.22	8	16
106.17	8	10
106.17	8	10
106.17	8	10
120.19	9	12
138.25	10	18
120.19	9	12
138.25	10	18
120.19	9	12
138.25	10	18
138.25	10	18
132.21	10	12
132.21	10	12
132.21	10	12
128.19	10	8
146.21	11	14
146.21	11	14
146.21	11	14
146.21	11	14
142.2	11	10
142.2	11	10
154.21	12	10
168.24	13	12
156.23	12	12
156.23	12	12
156.23	12	12
168.24	13	12
168.24	13	12
166.23	13	10
168.24	13	12
180.25	14	12
118	9	10
134	10	14
132	10	12

PROGRAM LOADER

```
800  REM  THIS PROGRAM IS A UTILITY TO STORE DATA IN A FILE
900  DIM MW(106),AC(106),AH(106)
910  FOR J = 1 TO 106
920  PRINT "COMPOUND";J
930  INPUT "MOLECULAR WT";MW(J)
940  INPUT "GATOMS CARBON";AC(J)
950  INPUT "GATOMS HYDROGEN";AH(J)
960  NEXT J
1000 DOS$ =  CHR$ (4)
2000  PRINT DOS$;"OPEN MATLBALDATA"
3000  PRINT DOS$;"WRITE MATLBALDATA"
4000  FOR J = 1 TO 106
5000  PRINT MW(J)
6000  NEXT J
7000  FOR J = 1 TO 106
8000  PRINT AC(J)
9000  NEXT J
10000  FOR J = 1 TO 106
11000  PRINT AH(J)
12000  NEXT J
12100  PRINT DOS$;"CLOSE MATLBALDATA"
12200  PRINT "THE DATA HAS BEEN STORED UNDER MATLBALDATA"
```

PROGRAM READER

```
4  REM  THIS PROGRAM IS A UTILITY TO LIST THE DATA IN MATLBA
LDATA
5  DIM MW(106),AC(106),AH(106)
10 DOS$ =  CHR$ (4)
20  PRINT DOS$;"OPEN MATLBALDATA"
30  PRINT DOS$;"READ MATLBALDATA"
40  FOR I = 1 TO 106
50  INPUT MW(I)
60  NEXT I
70  FOR I = 1 TO 106
80  INPUT AC(I)
90  NEXT I
100  FOR I = 1 TO 106
110  INPUT AH(I)
120  NEXT I
130  FOR I = 1 TO 106
135  PRINT DOS$;"CLOSE MATLBALDATA"
140  PRINT MW(I);"     ";AC(I);"      ";AH(I)
150  NEXT I
```

PROGRAM DATASTORE

```
10   DIM A(138)
20   INPUT "RUN FILE NAME ?";R$
30   INPUT "RUN NUMBER ?";A(1)
40   INPUT "PUMP TEMP/ DEG F ?";A(2)
50   INPUT "INITIAL TIME OF MATERIAL BALANCE ?";A(3)
60   INPUT "FINAL TIME OF MATERIAL BALANCE ?";A(4)
70   INPUT "INITIAL PUMP VOLUME/CC ?";A(5)
80   INPUT "FINAL PUMP VOLUME/CC ?";A(6)
90   INPUT "WT % OF TRANS-DECALIN ?";A(7)
100   INPUT "CIS-DECALIN ?";A(8)
110   INPUT "TETRALIN ?";A(9)
120   INPUT "FLUORENE ?";A(10)
130   INPUT "BAROMETRIC PRESSURE/ IN. HG ?";A(11)
140   INPUT "P CORRECTION/ IN. HG ?";A(12)
150   INPUT "H20 VAPOR PRESS/ IN. HG ?";A(13)
160   INPUT "WTM MIN/REV (INIT+FINAL/2)?";A(14)
170   INPUT "WTM TEMP (INIT+FINAL/2)?";A(15)
180   INPUT "GRAMS OF CATALYST ?";A(16)
190   INPUT "VOLUME OF CATALYST/CC ?";A(17)
200   INPUT "REACTOR PRESSURE/PSIG ?";A(18)
210   INPUT "REACTOR TEMPERATURE/DEG F?";A(19)
220   INPUT "INITIAL WTM CUBIC FEET ?";A(20)
230   INPUT "FINAL WTM CUBIC FEET ?";A(21)
240   INPUT "WTM TEMP/DEG F DURING M.B.?";A(22)
250   INPUT "GRAMS/HR IN COND A?";A(23)
260   INPUT "GRAMS/HR IN COND B?";A(24)
270   INPUT "ROOM TEMP/DEG F ?";A(25)
280   INPUT "GAS SAMPLE INJ VOLUME/CC ?";A(26)
290   INPUT "GC AREA COUNTS FOR GAS 2 ?";A(27)
300   INPUT "GC AREA COUNTS FOR GAS 3 ?";A(28)
310   INPUT "GC AREA COUNTS FOR GAS 4 ?";A(29)
320   INPUT "GC AREA COUNTS FOR GAS 5 ?";A(30)
330   INPUT "GC AREA COUNTS FOR GAS 6 ?";A(31)
340   INPUT "GC AREA COUNTS FOR GAS 7 ?";A(32)
350   FOR I = 33 TO 138
360   IF I > 85 THEN  GOTO 390
370   PRINT "COND A COMPOUND  ";I - 32
380   GOTO 400
390   PRINT "COND B COMPOUND  ";I - 85
400   INPUT "WT % ? ";A(I)
410   NEXT I
420   PRINT  CHR$ (4);"OPEN"R$",L10"
430   FOR J = 1 TO 138
440   PRINT  CHR$ (4);"WRITE"R$",R";J
450   PRINT A(J)
460   NEXT J
470   PRINT  CHR$ (4);"CLOSE"R$
480   PRINT "DATA IS FILED UNDER   ";R$
490   END
```

PROGRAM DATAPRTSI

```
10  DIM A(138)
20  INPUT "RUN FILE NAME ?";R$
30  PRINT  CHR$ (4);"OPEN"R$",L10"
40  FOR I = 1 TO 138
50  PRINT  CHR$ (4);"READ"R$",R";I
60  INPUT A(I)
70  NEXT I
80  PRINT  CHR$ (4);"CLOSE"R$
90 D$ =  CHR$ (13) +  CHR$ (4)
100  PRINT D$;"PR#1"
110  PRINT  CHR$ (9);"80N"
120  PRINT  CHR$ (9);"60P"
130  PRINT  CHR$ (9);"13L"
140  PRINT "RUN NUMBER =";A(1);"  INPUT DATA FOR M.B."
150  PRINT "DATA IS FILED UNDER   ";R$
160  PRINT "PUMP TEMP/ DEG K =";(A(2) + 459.67) / 1.8
170  PRINT "INITIAL TIME OF M. B./S  =";A(3) * 60; SPC( 5);
"FINAL TIME=";A(4) * 60
180  PRINT "INITIAL PUMP VOL/M3="; SPC( 3);A(5) / 1000000;
  "FINAL VOL/M3= ";A(6) / 1000000
190  PRINT "WT % OF TRANS-DECALIN =";A(7)
200  PRINT "CIS-DECALIN ="; SPC( 10);A(8)
210  PRINT "TETRALIN ="; SPC( 13);A(9)
220  PRINT "FLUORENE ="; SPC( 13);A(10)
230  PRINT "BAROMETRIC PRESSURE/ BARS   =";A(11) * 0.03386
240  PRINT "P CORRECTION/ BARS   ="; SPC( 9);A(12) * 0.0338
6
250  PRINT "H20 VAPOR PRESS/ BARS   ="; SPC( 5);A(13) * 0.0
3386
260  PRINT "WTM SEC/REV AVERAGE=";A(14) * 60;"  WTM TEMP/K=
";(A(15) + 459.67) / 1.8
270  PRINT "KGMS  OF CATALYST =";A(16) / 1000;"     VOLUME/
M3=";A(17) / 1000000
280  PRINT "REACTOR PRESS/BARS=";(A(18) + 14.696) * 0.06895
;"   REACTOR TEMP/K=";(A(19) + 459.67) / 1.8
290  PRINT "INITIAL WTM M3 = ";A(20) * 0.02832;"  FINAL M3
= ";A(21) * 0.02832
300  PRINT "WTM TEMP/DEG K DURING M.B.=";(A(22) + 459.67) /
1.8
310  PRINT "KGS/SEC  IN COND A=";A(23) * 2.778 * 10 ^  - 7;
"  KGS/SEC IN B = ";A(24) * 2.778 * 10 ^  - 7
320  PRINT "ROOM TEMP/DEG K =";(A(25) + 459.67) / 1.8
330  PRINT "GAS SAMPLE INJ VOLUME/M3 =";A(26) / 1000000
340  PRINT "GC AREA COUNTS, GAS 2 =";A(27);"  GAS 3 =";A(28
)
360  PRINT "GC AREA COUNTS, GAS 4 =";A(29);"  GAS 5 =";A(30
)
380  PRINT "GC AREA COUNTS, GAS 6 =";A(31);"  GAS 7 =";A(32
)
```

```
400  PRINT  SPC( 12);"WEIGHT % PRODUCT FROM G.C. ANALYSIS"
410  PRINT  SPC( 5);"    CONDENSER A                  CONDENSE
R  B"
420  PRINT  SPC( 5);"_____________________________    ____________
_____________"
430  PRINT  SPC( 5);"COMP#   WT%   COMP#  WT%   COMP#  WT%
  COMP#  WT%"
440  FOR I = 33 TO 58
450  HTAB 17: PRINT I - 32;
460  HTAB 22: PRINT A(I);
470  HTAB 30: PRINT I - 6;
480  HTAB 35: PRINT A(I + 26);
490  POKE 36,44: PRINT I - 32;
500  POKE 36,48: PRINT A(I + 53);
510  POKE 36,58: PRINT I - 6;
520  POKE 36,62: PRINT A(I + 79)
530  NEXT I
540  HTAB 30: PRINT "53";
550  HTAB 35: PRINT A(85);
560  POKE 36,58: PRINT "53";
570  POKE 36,62: PRINT A(138)
580  PRINT  CHR$ (4);"PR#0"
590  PRINT  CHR$ (4);"PR#3"
600  END
```

PROGRAM HJB.KINETIC.FIT

```
10  REM  HJB RATE CONSTANT PROGRAM FOR COMPLEX KINETIC MOD
EL OF HC OF FLUORENE/DECALIN SYSTEM
20  REM
30  DIM R(5,13,21),Y(5,13),C(5,13),G(22),S(22,22),A(22,22)
,RTIO(22),W(5,13)
40  REM  INPUT ARRAY SIZE AND TIME STEP
50  INPUT "NO. OF TIME INTERVALS ? ";P
60  INPUT " LENGTH OF SPACE TIME STEP/SEC ? ";H
70  INPUT "NO. OF EQUATIONS ? ";M
80  INPUT "NO. OF K'S ? ";N
90  REM  SUPPLY INITIAL CONCENTRATIONS
100  PRINT  CHR$ (4);"OPEN KINDAT730-2"
110  PRINT  CHR$ (4);"READ KINDAT730-2"
120  FOR I = 0 TO P
130  FOR J = 1 TO M
140  INPUT C(I,J)
150  NEXT J
160  NEXT I
170  PRINT  CHR$ (4);"CLOSE KINDAT730-2"
180  FOR I = 0 TO P
190  FOR J = 1 TO M
200 C(I,J) = C(I,J) * 0.00001
210  NEXT J
220  NEXT I
230  REM  BASED ON KINETIC MODEL INPUT R(I,J,K) FOR INTEGR
ATION STEP
240  REM  I=TIME INTERVAL, INCLUDING 0 (INITIAL)
250  REM  J=# OF EQUATIONS
260  REM  K=# OF RATE CONSTANTS
270  REM  GENERATE ZERO MATRIX

280  FOR I = 0 TO P
290  FOR J = 1 TO M
300  FOR K = 1 TO N
310 R(I,J,K) = 0
```

```
320  NEXT K
330  NEXT J
340  NEXT I
350  GOSUB 2000
500  REM  PERFORM INTEGRATION BY TRAP METHOD
510  FOR K = 1 TO N
520  FOR J = 1 TO M
530 SUM = 0
540  FOR I = 1 TO P
550 A = H * ((0.5 * R(0,J,K)) + SUM + (0.5 * R(I,J,K)))
560 SUM = SUM + R(I,J,K)
570 R(I,J,K) = A
580  NEXT I
590  NEXT J
600  NEXT K
610  REM  CALC Y(I,J)=C(I,J)-C(0,J)
620  FOR I = 1 TO P
630  FOR J = 1 TO M
640 Y(I,J) = C(I,J) - C(0,J)
645 W(I,J) = 1 /  ABS (Y(I,J))
650  NEXT J
660  NEXT I
670  REM  CALC CONSTANT VECTOR G(K)
680  FOR K = 1 TO N
690 G(K) = 0
700  FOR I = 1 TO P
710  FOR J = 1 TO M
720 G(K) = G(K) + (Y(I,J) * R(I,J,K) * (W(I,J) ^ 2))
730  NEXT J
740  NEXT I
750  NEXT K
760  REM  CALC COEFFICIENT MATRIX S(K,L)
770  FOR L = 1 TO N
780  FOR K = 1 TO N
790 S(K,L) = 0
800  FOR I = 1 TO P
810  FOR J = 1 TO M
820 S(K,L) = S(K,L) + (R(I,J,K) * R(I,J,L) * (W(I,J) ^ 2))

830  NEXT J
840  NEXT I
850  NEXT K
860  NEXT L
870  REM  SEND S(K,L) AND G(K) TO GAUSS JORDAN SOLUTION FO
R K(K)'S
880  REM  SOLUTION OF A SET OF LINEAR EQUATIONS BY GAUSS-J
ORDAN ELIMINATION
890  REM    NUMBER OF VARIABLES = N
900 CP$ = "N"
910 CF = 0
920  IF CP$ = "Y" THEN CF = 1
930 N1 = N
940 N2 = N + 1
```

```
950  FOR I = 1 TO N1
960  FOR J = 1 TO N1
970 A(I,J) = S(I,J)
980  NEXT J
990  NEXT I
1000  FOR I = 1 TO N1
1010 A(I,N2) = G(I)
1020  NEXT I
1030  REM  GAUSS-JORDAN ELIMINATION STEP
1040  FOR K = 1 TO N1
1050  IF CF = 0 GOTO 1070
1060  PRINT "FOR ROW:",K
1070  GOSUB 1320: REM  PIVOTING SUBROUTINE
1080  IF IX = 2 THEN 1290: REM  STOP THE PROGRAM
1090 S = A(K,K)
1100  FOR J = K TO N2
1110 A(K,J) = A(K,J) / S
1120  NEXT J
1130  FOR I = 1 TO N1
1140  IF I = K THEN 1200
1150 J = K
1160 S = A(I,K)
1170 A(I,J) = A(I,J) - S * A(K,J)
1180 J = J + 1
1190  IF J <  = N2 THEN 1170
1200  REM  CONTINUE
1210  NEXT I
1220  NEXT K
1230  REM  SOLUTION PRINTOUT HERE A(1,N2)...A(2,N2)...A(N1
,N2)
1235  PRINT  CHR$ (7)
1236  PRINT  CHR$ (7)
1237  PRINT  CHR$ (7)
1243  PRINT  CHR$ (4);"PR#1"
1244  PRINT  CHR$ (9);"80N"
1245  PRINT  CHR$ (9);"10L"
1246  PRINT "SOLUTION TO THE EQUATIONS IS :"
1250  FOR I = 1 TO N1
1260  PRINT "K";I;" = ";A(I,N2)
1270  NEXT I
1275  PRINT  CHR$ (4);"PR#0"
1276  PRINT  CHR$ (4);"PR#3"
1280  GOTO 1310
1290  PRINT "THERE IS A ROW WITH ZERO ELEMENTS"
1300  PRINT "THE PROGRAM IS TERMINATED"
1310  END
1320  REM  THIS SUBROUTINE WILL SELECT THE BEST PIVOTING R
OW BY THE TERM SCALED PIVOTING METHOD
1330  REM  NR.... NUMBER OF ROWS
1340  REM  NCAM.. NUMBER OF COLUMNS
1350  REM  NC.... NUMBER OF COLUMN DELETING THE AUGMENTED
COLUMN
1360 NR = N
```

```
1370 IX = 1: REM  INITIALIZE THE FLAG
1380 NC = N2 - 1
1390  REM  CHECKING IF THIS IS THE LAST ROW IN THE MATRIX
1400  IF K = NC THEN  RETURN
1410  REM  SELECTING THE LARGEST MEMBER OF EACH ROW
1420  FOR IS = K TO NR
1430 JS = K
1440 BG =  ABS (A(IS,K))
1450 JD = JS + 1
1460  FOR JJ = JD TO NC
1470 AX =  ABS (A(IS,JJ))
1480  IF AX > BG THEN BG = AX
1490  NEXT JJ
1500  REM  CHECK IF THE LARGEST NUMBER IS ZERO
1510  IF BG < 1 * 10 ^  - 20 THEN 1730: REM  SET FLAG AND
RETURN
1520 RTIO(IS) = A(IS,K) / BG
1530  NEXT IS
1540 IS = K
1550 IR = IS
1560 PV =  ABS (RTIO(IS))
1570 JD = IS + 1
1580  FOR JS = JD TO NR
1590 BT =  ABS (RTIO(JS))
1600  IF BT > PV THEN 1620
1610  GOTO 1640
1620 IR = JS
1630 PV = BT
1640  NEXT JS
1650  IF IR = K THEN  RETURN
1660 IK = IR
1670  FOR JM = K TO N2
1680 DM = A(K,JM)
1690 A(K,JM) = A(IK,JM)
1700 A(IK,JM) = DM
1710  NEXT JM
1720  RETURN
1730 IX = 2
1740  RETURN
2000  REM  COMPUTE R(I,J,K) FOR INTEGRATION
2010  REM  LIST EQUATIONS IN THIS SUBROUTINE
2020  FOR I = 0 TO P
2030 R(I,1,4) = C(I,9)
2040 R(I,1,8) = C(I,5)
2050 R(I,1,11) = C(I,5)
2060 R(I,1,13) = C(I,7)
2070 R(I,1,19) = C(I,8)
2080 R(I,2,8) = C(I,5)
2090 R(I,2,9) = C(I,3)
2100 R(I,2,10) =  - C(I,2)
2120 R(I,3,9) =  - C(I,3)
2130 R(I,3,10) = C(I,2)
2140 R(I,3,11) = C(I,5)
```

```
2150 R(I,3,12) =  - C(I,3)
2155 R(I,3,13) = C(I,7)
2160 R(I,4,4) = C(I,9)
2170 R(I,4,1) = 2 * C(I,7) * C(I,12)
2180 R(I,4,12) = C(I,3)
2190 R(I,4,19) = C(I,8)
2200 R(I,5,7) =  - C(I,5)
2210 R(I,5,8) =  - C(I,5)
2220 R(I,5,11) =  - C(I,5)
2230 R(I,5,15) =  - C(I,5)
2240 R(I,5,14) = C(I,7)
2250 R(I,6,16) =  - C(I,6)
2260 R(I,6,17) = C(I,7)
2270 R(I,7,13) =  - C(I,7)
2280 R(I,7,14) =  - C(I,7)
2290 R(I,7,15) = C(I,5)
2300 R(I,7,16) = C(I,6)
2310 R(I,7,17) =  - C(I,7)
2320 R(I,7,18) =  - C(I,7)
2330 R(I,7,1) =  - C(I,7) * C(I,12)
2340 R(I,7,2) =  - C(I,7) * C(I,12)
2350 R(I,7,3) =  - C(I,7) * C(I,12)
2360 R(I,8,5) =  - C(I,8)
2370 R(I,8,6) = C(I,9)
2380 R(I,8,18) = C(I,7)
2390 R(I,8,19) =  - C(I,8)
2400 R(I,8,20) =  - C(I,8)
2410 R(I,8,1) = C(I,7) * C(I,12)
2420 R(I,8,2) = C(I,7) * C(I,12)
2430 R(I,8,3) = C(I,7) * C(I,12)
2440 R(I,9,3) = C(I,7) * C(I,12)
2450 R(I,9,4) =  - C(I,9)
2460 R(I,9,5) = C(I,8)
2470 R(I,9,6) =  - C(I,9)
2480 R(I,9,7) = C(I,5)
2490 R(I,10,20) = C(I,8)
2500 R(I,11,2) = C(I,7) * C(I,12)
2510 R(I,12,1) =  - C(I,7) * C(I,12)
2520 R(I,12,2) =  - C(I,7) * C(I,12)
2530 R(I,12,3) =  - C(I,7) * C(I,12)
2600  NEXT I
2610  RETURN
```

PROGRAM KINDAT.10.2

```
10  REM  KINDATSTORE PROGRAM FOR PUTTING CONC ON DISK
20  REM
30  DIM C(5,12)
40  FOR I = 0 TO 5
50  FOR J = 1 TO 12
60  PRINT "TIME= ";I;"  COMPOUND=  ";J
70  INPUT C(I,J)
80  NEXT J
90  NEXT I
100  PRINT  CHR$ (4);"OPEN KINDAT730-2"
110  PRINT  CHR$ (4);"WRITE KINDAT730-2"
120  FOR I = 0 TO 5
130  FOR J = 1 TO 12
140  PRINT C(I,J)
150  NEXT J
160  NEXT I
170  PRINT  CHR$ (4);"CLOSE KINDAT730-2"
175  PRINT  CHR$ (4);"OPEN KINDAT730-2"
177  PRINT  CHR$ (4);"READ KINDAT730-2"
180  FOR I = 0 TO 5
190  FOR J = 1 TO 12
200  INPUT C(I,J)
210  NEXT J
220  NEXT I
230  PRINT  CHR$ (4);"CLOSE KINDAT730-2"
240  FOR I = 0 TO 5
250  FOR J = 1 TO 12
260  PRINT C(I,J)
270  NEXT J
280  NEXT I
290  END
```

DATASET KINDAT730-2

0
0
0
.567
.204
217.51
341.67
8.05
1.15
1.36
6.24
104.1
33
11.5
5
20
12.5
222
246.7
6
12.5
13
11.54
69.1
78
29.5
6.5
52.3
23.5
210
168.3
6
21
21
13.38
52.2
110
42
10.1
82
37
209
110
6.6
35
25
15.23
49.1
113
43.5
10.3
92.3
44.5
196
71.7
6.4
40
28
17.38
49.35
116
45.5
10.6
103.9
52
184
33.3
6
46
31
19.23
49.7

PROGRAM FIT730

```
C     730 F RUN
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION P(30),STEP(30),C(5,12),CO(12)
      DO 1 J=1,12
    1 READ(5,200) CO(J)
      DO 2 I=1,5
      DO 2 J=1,12
    2 READ(5,200) C(I,J)
      DO 3 I=1,5
      DO 3 J=1,12
    3 C(I,J)=C(I,J)*1.0D-5
      DO 4 J=1,12
      CO(J)=CO(J)*1.0D-5
    4 WRITE(6,300) CO(J)
      DO 5 I=1,5
      DO 5 J=1,12
    5 WRITE(6,300) C(I,J)
C     INITIAL GUESSES FOR RATE CONSTANTS
      P(1)=25.21
      P(2)=20.80
      P(3)=.7172D-2
      P(4)=.3162D-20
      P(5)=2.9058
      P(6)=.7875
      P(7)=.2403
      P(8)=.279D-16
      P(9)=13.67
      P(10)=3.0888
      P(11)=.5153D-17
      P(12)=.07805
      P(13)=.07566
      P(14)=.07163
      P(15)=.11431D-16
      P(16)=.09225
      P(17)=.07692
      P(18)=.08373
      P(19)=2.0228
      P(20)=1.1645
C     INITIAL STEP SIZE FOR EACH RATE CONSTANT
      STEP(1)=1.0
      STEP(2)=1.0
      STEP(3)=1.0D-4
      STEP(4)=1.0D-22
      STEP(5)=1.0D-1
      STEP(6)=1.0D-2
      STEP(7)=1.0D-2
      STEP(8)=1.0D-18
      STEP(9)=1.0
      STEP(10)=1.0D-1
      STEP(11)=1.0D-19
      STEP(12)=1.0D-3
```

```
      STEP(13)=1.0D-3
      STEP(14)=1.0D-3
      STEP(15)=1.0D-18
      STEP(16)=1.0D-3
      STEP(17)=1.0D-3
      STEP(18)=1.0D-3
      STEP(19)=1.0D-1
      STEP(20)=1.0D-1
      CALL PATERN(20,P,STEP,2,2,COST,C,CO)
  200 FORMAT(D10.5)
  300 FORMAT(10X,D10.5)
      STOP
      END
      SUBROUTINE PATERN(NP,P,STEP,NPASS,IO,COST,C,CO)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION P(30),STEP(30),B1(100),B2(100),T(100),S(100)
      DIMENSION C(5,12),CO(12)
C     VECTORS B1,B2,T,S NEED ONLY BE DIMENSIONED BY A NUMBER
C     EQUAL TO THE NUMBER OF PARAMETERS NP
C     STARTING POINT
      NRD =NPASS
      L=1
      ICK = 2
      ITTER = 0
      DO 5 I=1,NP
      B1(I) = P(I)
      B2(I) = P(I)
      T(I) = P(I)
    5 S(I) = STEP(I)*10.
C     INITIAL BOUNDARY CHECK AND COST EVALUATION
      CALL BOUNDS(P,IOUT)
      IF(IOUT.LE.0) GO TO 10
      IF(IO.LE.0) GO TO 6
      WRITE(6,1005)
      WRITE(6,1000) (J,P(J),J=1,NP)
    6 RETURN
   10 CALL PROC(P,C1,C,CO)
      IF(IO.LE.1) GO TO 11
      WRITE(6,1001) ITTER,C1
      WRITE(6,1000) (J,P(J),J=1,NP)
C     BEGINNING OF PATTERN SEARCH STRATEGY
   11 DO 99 INRD = 1,NRD
      DO 12 I=1,NP
   12 S(I) = S(I)/10.
      IF(IO.LE.1) GO TO 20
      WRITE(6,1003)
      WRITE(6,1000) (J,S(J),J=1,NP)
   20 IFAIL = 0
C     PERTURBATION ABOUT T
      DO 30 I=1,NP
      IC = 0
   21 P(I) = T(I) + S(I)
      IC = IC + 1
      CALL BOUNDS(P,IOUT)
      IF(IOUT.GT.0)GO TO 23
      CALL PROC(P,C2,C,CO)
      L = L+1
      IF(IO.LT.3) GO TO 22
      WRITE(6,1002)L,C2
      WRITE(6,1000) (J,P(J),J=1,NP)
C     IF(L.GT.100) RETURN
```

```
   22 IF(C1-C2) 23,23,25
   23 IF(IC.GE.2) GO TO 24
      S(I) = -S(I)
      GO TO 21
   24 IFAIL = IFAIL + 1
      P(I) = T(I)
      GO TO 30
   25 T(I) = P(I)
      C1 = C2
   30 CONTINUE
      IF(IFAIL.LT.NP) GO TO 35
      IF(ICK.EQ.2) GO TO 90
      IF(ICK.EQ.1) GO TO 35
      CALL PROC(T,C2,C,CO)
      L = L+1
      IF(IO.LT.3) GO TO 31
      WRITE(6,1002) L,C2
      WRITE(6,1000) (J,T(J),J=1,NP)
C     IF(L.GT.50) RETURN
   31 IF(C1-C2) 32,34,34
   32 ICK = 1
      DO 33 I=1,NP
      B1(I) = B2(I)
      P(I) = B2(I)
   33 T(I) = B2(I)
      GO TO 20
   34 C1 = C2
   35 IB1 = 0
      DO 39 I=1,NP
      B2(I) = T(I)
      IF (DABS(B1(I)-B2(I)).LT.0.01*DABS(S(I))) IB1 = IB1 + 1
   39 CONTINUE
      IF(IB1.EQ.NP) GO TO 90
      ICK = 0
      ITTER = ITTER + 1
      IF(IO.LT.2) GO TO 40
      WRITE(6,1001)ITTER,C1
      WRITE(6,1000) (J,T(J),J=1,NP)
C      ACCELERATION STEP
   40 SJ = 1.0
      DO 45 II = 1,11
      DO 42 I = 1,NP
      T(I) = B2(I) +SJ*(B2(I)-B1(I))
   42 P(I) = T(I)
      SJ = SJ - 0.1
      CALL BOUNDS(T,IOUT)
      IF(IOUT.LT.1)GO TO 46
      IF(II.EQ.11) ICK = 1
   45 CONTINUE
   46 DO 47 I=1,NP
   47 B1(I) = B2(I)
      GO TO 20
   90 DO 91 I=1,NP
   91 T(I)= B2(I)
   99 CONTINUE
      DO 100 I=1,NP
  100 P(I)=T(I)
      COST = C1
      IF(IO.LE.0) RETURN
      WRITE(6,1004) L,C1
      WRITE(6,1000) (J,P(J),J=1,NP)
```

```
      RETURN
 1000 FORMAT(10X,5(I7,3X,D13.6)/)
 1001 FORMAT(//1X,'ITTERATION NO. ',I5/5X,5HCOST= ,D15.6,20X,
     110HPARAMETERS)
 1002 FORMAT(10X,'NO.  ',I4, 8X,5HCOST=,D15.6)
 1003 FORMAT(/1X,'STEP SIZE FOR EACH PARAMETER ' )
 1004 FORMAT(1H1,13HANSWERS AFTER ,I3,2X,23HFUNCTIONAL EVALUATIONS  //
     1    5X,5HCOST=,D15.6,20X,18HOPTIMAL PARAMETERS )
 1005 FORMAT(1H1,35HINITIAL PARAMETERS OUT OF BOUNDS      )
      END
C
C
      SUBROUTINE BOUNDS(P,IOUT)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION P(30)
      IOUT = 0
      IF(P(1).LT.0.0) IOUT=1
      IF(P(2).LT.0.0) IOUT=1
      IF(P(3).LT.0.0) IOUT=1
      IF(P(4).LT.0.0) IOUT=1
      IF(P(5).LT.0.0) IOUT=1
      IF(P(6).LT.0.0) IOUT=1
      IF(P(7).LT.0.0) IOUT=1
      IF(P(8).LT.0.0) IOUT=1
      IF(P(9).LT.0.0) IOUT=1
      IF(P(10).LT.0.0) IOUT=1
      IF(P(11).LT.0.0) IOUT=1
      IF(P(12).LT.0.0) IOUT=1
      IF(P(13).LT.0.0) IOUT=1
      IF(P(14).LT.0.0) IOUT=1
      IF(P(15).LT.0.0) IOUT=1
      IF(P(16).LT.0.0) IOUT=1
      IF(P(17).LT.0.0) IOUT=1
      IF(P(18).LT.0.0) IOUT=1
      IF(P(19).LT.0.0) IOUT=1
      IF(P(20).LT.0.0) IOUT=1
      RETURN
      END
C
C
      SUBROUTINE PROC(P,COST,C,CO)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION P(30),Y1(5,12),Y2(5,12),R(5,12,30)
      DIMENSION W(5,12),C(5,12),CO(12),RO(12,30)
      N=20
      DO 4 I=1,5
      DO 4 J=1,12
      DO 4 K=1,N
    4 R(I,J,K)=0.D0
      DO 20 J=1,12
      DO 20 K=1,N
   20 RO(J,K)=0.D0
C     INSERT EQUATIONS FOR RO(J,K) AND R(I,J,K)
C     BO FIRST AS RO(1,3)=CO(9)
C     R NEXT IN LOOP AS R(1,Y,Z)=C(I,Q)
      RO(1,19)=CO(8)
      RO(1,4)=CO(9)
      RO(1,8)=CO(5)
      RO(1,11)=CO(5)
      RO(1,13)=CO(7)
      RO(2,8)=CO(5)
```

```
      RO(2,9)=CO(3)
      RO(2,10)=-CO(2)
      RO(3,9)=-CO(3)
      RO(3,10)=CO(2)
      RO(3,11)=CO(5)
      RO(3,12)=-CO(3)
      RO(3,13)=CO(7)
      RO(4,1)=2.0D0*CO(7)*CO(12)
      RO(4,4)=CO(9)
      RO(4,12)=CO(3)
      RO(4,19)=CO(8)
      RO(5,7)=-CO(5)
      RO(5,8)=-CO(5)
      RO(5,11)=-CO(5)
      RO(5,15)=-CO(5)
      RO(5,14)=CO(7)
      RO(6,16)=-CO(6)
      RO(6,17)=CO(7)
      RO(7,1)=-CO(7)*CO(12)
      RO(7,2)=-CO(7)*CO(12)
      RO(7,3)=-CO(7)*CO(12)
      RO(7,13)=-CO(7)
      RO(7,14)=-CO(7)
      RO(7,15)=CO(5)
      RO(7,16)=CO(6)
      RO(7,17)=-CO(7)
      RO(7,18)=-CO(7)
      RO(8,5)=-CO(8)
      RO(8,6)=CO(9)
      RO(8,18)=CO(7)
      RO(8,19)=-CO(8)
      RO(8,20)=-CO(8)
      RO(8,1)=CO(7)*CO(12)
      RO(8,2)=CO(7)*CO(12)
      RO(8,3)=CO(7)*CO(12)
      RO(9,3)=CO(7)*CO(12)
      RO(9,4)=-CO(9)
      RO(9,5)=CO(8)
      RO(9,6)=-CO(9)
      RO(9,7)=CO(5)
      RO(10,20)=CO(8)
      RO(11,2)=CO(7)*CO(12)
      RO(12,1)=-CO(7)*CO(12)
      RO(12,2)=-CO(7)*CO(12)
      RO(12,3)=-CO(7)*CO(12)
      DO 5 I=1,5
      R(I,1,19)=C(I,8)
      R(I,1,4)=C(I,9)
      R(I,1,8)=C(I,5)
      R(I,1,11)=C(I,5)
      R(I,1,13)=C(I,7)
      R(I,2,8)=C(I,5)
      R(I,2,9)=C(I,3)
      R(I,2,10)=-C(I,2)
      R(I,3,9)=-C(I,3)
      R(I,3,10)=C(I,2)
      R(I,3,11)=C(I,5)
      R(I,3,12)=-C(I,3)
      R(I,3,13)=C(I,7)
      R(I,4,1)=2.0D0*C(I,7)*C(I,12)
      R(I,4,4)=C(I,9)
```

```
      R(I,4,12)=C(I,3)
      R(I,4,19)=C(I,8)
      R(I,5,7)=-C(I,5)
      R(I,5,8)=-C(I,5)
      R(I,5,11)=-C(I,5)
      R(I,5,15)=-C(I,5)
      R(I,5,14)=C(I,7)
      R(I,6,16)=-C(I,6)
      R(I,6,17)=C(I,7)
      R(I,7,1)=-C(I,7)*C(I,12)
      R(I,7,2)=-C(I,7)*C(I,12)
      R(I,7,3)=-C(I,7)*C(I,12)
      R(I,7,13)=-C(I,7)
      R(I,7,14)=-C(I,7)
      R(I,7,15)=C(I,5)
      R(I,7,16)=C(I,6)
      R(I,7,17)=-C(I,7)
      R(I,7,18)=-C(I,7)
      R(I,8,5)=-C(I,8)
      R(I,8,6)=C(I,9)
      R(I,8,18)=C(I,7)
      R(I,8,19)=-C(I,8)
      R(I,8,20)=-C(I,8)
      R(I,8,1)=C(I,7)*C(I,12)
      R(I,8,2)=C(I,7)*C(I,12)
      R(I,8,3)=C(I,7)*C(I,12)
      R(I,9,3)=C(I,7)*C(I,12)
      R(I,9,4)=-C(I,9)
      R(I,9,5)=C(I,8)
      R(I,9,6)=-C(I,9)
      R(I,9,7)=C(I,5)
      R(I,10,20)=C(I,8)
      R(I,11,2)=C(I,7)*C(I,12)
      R(I,12,1)=-C(I,7)*C(I,12)
      R(I,12,2)=-C(I,7)*C(I,12)
    5 R(I,12,3)=-C(I,7)*C(I,12)
C     NOW PERFORM INTEGRATION BY TRAPEZOID RULE
C     STEP IS 1 SECOND: H=1.0
      DO 6 K=1,N
      DO 6 J=1,12
      SUM=0.D0
      DO 6 I=1,5
      A=1.0D0*((0.5D0*RO(J,K))+SUM+(0.5D0*P(I,J,K)))
      SUM=SUM+P(I,J,K)
    6 R(I,J,K)=A
C     CALC THE ACTUAL MEASURED Y1 VALUE
      DO 7 I=1,5
      DO 7 J=1,12
      Y1(I,J)=C(I,J)-CO(J)
    7 W(I,J)=1.0D0/DABS(Y1(I,J))
      DO 8 I=1,5
      DO 8 J=1,12
      Y2(I,J)=0.D0
      DO 8 K=1,N
    8 Y2(I,J)=Y2(I,J)+(P(K)*R(I,J,K))
      COST=0.D0
      DO 9 I=1,5
      DO 9 J=1,12
    9 COST=COST+(((Y1(I,J)-Y2(I,J))*W(I,J))**2)
      RETURN
      END
```

```
//
0.0
0.0
0.0
.567
.204
217.51
341.67
8.05
1.15
1.36
6.24
104.10
33.0
11.5
5.0
20.0
12.5
222.0
246.7
6.0
12.5
13.0
11.54
69.1
78.0
29.5
6.5
52.3
23.5
210.0
168.3
6.0
21.0
21.0
13.38
52.2
110.0
42.0
10.1
82.0
37.0
209.0
110.0
6.6
35.0
25.0
15.23
49.1
113.0
43.5
10.3
92.3
44.5
196.0
71.7
6.4
40.0
28.0
17.38
49.35
```

```
116.0
45.5
10.6
103.9
52.0
184.0
33.3
6.0
46.0
31.0
19.23
49.7
//
```

PROGRAM ACTIV

```
C     ACTIVATION ENERGY ROUTINE BASED ON 730 F DATA
C     AND THE TEMPERATURE RUN SERIES DATA
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION P(30),STEP(30)
      COMMON C(12,1,12),CO(12,12),BA(20)
      DO 1 L=1,12
      DO 1 J=1,12
    1 READ(5,200) CO(L,J)
      DO 2 L=1,12
      DO 2 J=1,12
    2 READ(5,200) C(L,1,J)
      DO 3 L=1,12
      DO 3 J=1,12
    3 C(L,1,J)=C(L,1,J)*1.0D-5
      DO 4 L=1,12
      DO 4 J=1,12
      CO(L,J)=CO(L,J)*1.0D-5
    4 WRITE(6,300) CO(L,J)
      DO 5 L=1,12
      DO 5 J=1,12
    5 WRITE(6,300) C(L,1,J)
      DO 25 K=1,20
   25 READ(5,200) BA(K)
      BA(4)=0.3162D-20
      BA(8)=0.279D-16
      BA(11)=0.5153D-17
      BA(15)=0.1143D-16
      DO 35 K=1,20
   35 WRITE(6,400) BA(K)
C     INITIAL GUESSES FOR ACTIVATION ENERGY KCAL/KGMOLE
      P(1)=13791.
      P(2)=10186.0
      P(3)=14685.
      P(4)=19773.
      P(5)=19638.
      P(6)=.70D-11
      P(7)=8251.0
      P(8)=10000.
      P(9)=19028.
      P(10)=8407.0
      P(11)=10000.
      P(12)=134576.
      P(13)=28438.
      P(14)=.4100D-19
      P(15)=10000.
      P(16)=16400.
      P(17)=8873.0
      P(18)=36427.
      P(19)=22918.
      P(20)=23863.
C     INITIAL STEP SIZE FOR EACH RATE CONSTANT
      STEP(1)=100.
```

```
      STEP(2) =100.
      STEP(3) =100.
      STEP(4) =100.
      STEP(5) =100.
      STEP(6) =1.0D-13
      STEP(7) =100.
      STEP(8) =100.
      STEP(9) =100.
      STEP(10) =100.
      STEP(11) =100.
      STEP(12) =1000.
      STEP(13) =1000.
      STEP(14) =1.0D-21
      STEP(15) =100.
      STEP(16) =100.
      STEP(17) =100.
      STEP(18) =100.
      STEP(19) =100.
      STEP(20) =100.
      CALL PATERN(20,P,STEP,3,2,COST)
  200 FORMAT(D12.5)
  300 FORMAT(10X,D10.5)
  400 FORMAT(10X,D20.10)
      STOP
      END
      SUBROUTINE PATERN(NP,P,STEP,NPASS,IO,COST)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION P(30),STEP(30),B1(100),B2(100),T(100),S(100)
      COMMON C(12,1,12),CC(12,12),BA(20)
C     VECTORS B1,B2,T,S NEED ONLY BE DIMENSIONED BY A NUMBER
C     EQUAL TO THE NUMBER OF PARAMETERS NP
C     STARTING POINT
      NRD =NPASS
      L=1
      ICK = 2
      ITTER = 0
      DO 5 I=1,NP
      B1(I) = P(I)
      B2(I) = P(I)
      T(I) = P(I)
    5 S(I) = STEP(I)*10.
C     INITIAL BOUNDARY CHECK AND COST EVALUATION
      CALL BOUNDS(P,IOUT)
      IF(IOUT.LE.0) GO TO 10
      IF(IO.LE.0) GO TO 6
      WRITE(6,1005)
      WRITE(6,1000) (J,P(J),J=1,NP)
    6 RETURN
   10 CALL PROC(P,C1)
      IF(IO.LE.1)GO TO 11
      WRITE(6,1001)ITTER,C1
      WRITE(6,1000) (J,P(J),J=1,NP)
C     BEGINNING OF PATTERN SEARCH STRATEGY
   11 DO 99 INRD = 1,NRD
      DO 12 I=1,NP
   12 S(I) = S(I)/10.
      IF(IO.LE.1) GO TO 20
      WRITE(6,1003)
      WRITE(6,1000) (J,S(J),J=1,NP)
   20 IFAIL = 0
C     PERTURBATION ABOUT T
```

```
      DO 30 I=1,NP
      IC = 0
   21 P(I) = T(I) + S(I)
      IC = IC + 1
      CALL BOUNDS(P,IOUT)
      IF(IOUT.GT.0) GO TO 23
      CALL PROC(P,C2)
      L = L+1
      IF(IO.LT.3) GO TO 22
      WRITE(6,1002) L,C2
      WRITE(6,1000) (J,P(J),J=1,NP)
C     IF(L.GT.100) RETURN
   22 IF(C1-C2) 23,23,25
   23 IF(IC.GE.2) GO TO 24
      S(I) = -S(I)
      GO TO 21
   24 IFAIL = IFAIL + 1
      P(I) = T(I)
      GO TO 30
   25 T(I) = P(I)
      C1 = C2
   30 CONTINUE
      IF(IFAIL.LT.NP) GO TO 35
      IF(ICK.EQ.2) GO TO 90
      IF(ICK.EQ.1) GO TO 35
      CALL PROC(T,C2,C,CO)
      L = L+1
      IF(IO.LT.3) GO TO 31
      WRITE(6,1002) L,C2
      WRITE(6,1000) (J,T(J),J=1,NP)
C     IF(L.GT.50) RETURN
   31 IF(C1-C2) 32,34,34
   32 ICK = 1
      DO 33 I=1,NP
      B1(I) = B2(I)
      P(I) = B2(I)
   33 T(I) = B2(I)
      GO TO 20
   34 C1 = C2
   35 IB1 = 0
      DO 39 I=1,NP
      B2(I) = T(I)
      IF (DABS(B1(I)-B2(I)).LT.0.01*DABS(S(I))) IB1 = IB1 + 1
   39 CONTINUE
      IF(IB1.EQ.NP) GO TO 90
      ICK = 0
      ITTER = ITTER + 1
      IF(IO.LT.2) GO TO 40
      WRITE(6,1001) ITTER,C1
      WRITE(6,1000) (J,T(J),J=1,NP)
C      ACCELERATION STEP
   40 SJ = 1.0
      DO 45 II = 1,11
      DO 42 I = 1,NP
      T(I) = B2(I) +SJ*(B2(I)-B1(I))
   42 P(I) = T(I)
      SJ = SJ - 0.1
      CALL BOUNDS(T,IOUT)
      IF(IOUT.LT.1) GO TO 46
      IF(II.EQ.11) ICK = 1
   45 CONTINUE
```

```
   46 DO 47 I=1,NP
   47 B1(I) = B2(I)
      GO TO 20
   90 DO 91 I=1,NP
   91 T(I)= B2(I)
   99 CONTINUE
      DO 100 I=1,NP
  100 P(I)=T(I)
      COST = C1
      IF(IO.LE.0) RETURN
      WRITE(6,1004) L,C1
      WRITE(6,1000)  (J,P(J),J=1,NP)
      RETURN
 1000 FORMAT(10X,5(I7,3X,D13.6)/)
 1001 FORMAT(//1X,'ITTERATION NO. ',I5/5X,5HCOST= ,D15.6,20X,
     110HPARAMETERS)
 1002 FORMAT(10X,'NO.  ',I4, 8X,5HCOST=,D15.6)
 1003 FORMAT(/1X,'STEP SIZE FOR EACH PARAMETER ' )
 1004 FORMAT(1H1,13HANSWERS AFTER ,I3,2X,23HFUNCTIONAL EVALUATIONS  //
     1    5X,5HCOST=,D15.6,20X,18HOPTIMAL PARAMETERS )
 1005 FORMAT(1H1,35HINITIAL PARAMETERS OUT OF BOUNDS      )
      END


      SUBROUTINE BOUNDS(P,IOUT)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION P(30)
      IOUT = 0
      IF(P(1).LT.0.0) IOUT=1
      IF(P(2).LT.0.0) IOUT=1
      IF(P(3).LT.0.0) IOUT=1
      IF(P(4).LT.0.0) IOUT=1
      IF(P(5).LT.0.0) IOUT=1
      IF(P(6).LT.0.0) IOUT=1
      IF(P(7).LT.0.0) IOUT=1
      IF(P(8).LT.0.0) IOUT=1
      IF(P(9).LT.0.0) IOUT=1
      IF(P(10).LT.0.0)  IOUT=1
      IF(P(11).LT.0.0)  IOUT=1
      IF(P(12).LT.0.0)  IOUT=1
      IF(P(13).LT.0.0)  IOUT=1
      IF(P(14).LT.0.0)  IOUT=1
      IF(P(15).LT.0.0)  IOUT=1
      IF(P(16).LT.0.0)  IOUT=1
      IF(P(17).LT.0.0)  IOUT=1
      IF(P(18).LT.0.0)  IOUT=1
      IF(P(19).LT.0.0)  IOUT=1
      IF(P(20).LT.0.0)  IOUT=1
      IF(P(1).GT.200000.0)  IOUT=1
      IF(P(2).GT.200000.0)  IOUT=1
      IF(P(3).GT.200000.0)  IOUT=1
      IF(P(4).GT.200000.0)  IOUT=1
      IF(P(5).GT.200000.0)  IOUT=1
      IF(P(6).GT.200000.0)  IOUT=1
      IF(P(7).GT.200000.0)  IOUT=1
      IF(P(8).GT.200000.0)  IOUT=1
      IF(P(9).GT.200000.0)  IOUT=1
      IF(P(10).GT.200000.0)  IOUT=1
      IF(P(11).GT.200000.0)  IOUT=1
      IF(P(12).GT.200000.0)  IOUT=1
      IF(P(13).GT.200000.0)  IOUT=1
```

```
      IF(P(14).GT.200000.0)  IOUT=1
      IF(P(15).GT.200000.0)  IOUT=1
      IF(P(16).GT.200000.0)  IOUT=1
      IF(P(17).GT.200000.0)  IOUT=1
      IF(P(18).GT.200000.0)  IOUT=1
      IF(P(19).GT.200000.0)  IOUT=1
      IF(P(20).GT.200000.0)  IOUT=1
      RETURN
      END
C
C
      SUBROUTINE PROC(P,COST)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON C(12,1,12),CO(12,12),RA(20)
      DIMENSION P(30),Y1(12,1,12),Y2(12,1,12),R(12,1,12,20)
      DIMENSION W(12,1,12),RO(12,12,20),A(20),T(12),RG(12,20)
      N=20
      DO 4 L=1,12
      DO 4 J=1,12
      DO 4 K=1,N
      RO(L,J,K)=0.D0
    4 R(L,1,J,K)=0.D0
C     INSERT EQUATIONS FOR RO(L,J,K) AND R(L,1,J,K)
C     RO FIRST AS RO(1,3)=CO(9)
C     R NEXT IN LOOP AS R(I,Y,Z)=C(I,Q)
      DO 50 L=1,12
      RO(L,1,19)=CO(L,8)
      RO(L,1,4)=CO(L,9)
      RO(L,1,8)=CO(L,5)
      RO(L,1,11)=CO(L,5)
      RO(L,1,13)=CO(L,7)
      RO(L,2,8)=CO(L,5)
      RO(L,2,9)=CO(L,3)
      RO(L,2,10)=-CO(L,2)
      RO(L,3,9)=-CO(L,3)
      RO(L,3,10)=CO(L,2)
      RO(L,3,11)=CO(L,5)
      RO(L,3,12)=-CO(L,3)
      RO(L,3,13)=CO(L,7)
      RO(L,4,1)=2.0D0*CO(L,7)*CO(L,12)
      RO(L,4,4)=CO(L,9)
      RO(L,4,12)=CO(L,3)
      RO(L,4,19)=CO(L,8)
      RO(L,5,7)=-CO(L,5)
      RO(L,5,8)=-CO(L,5)
      RO(L,5,11)=-CO(L,5)
      RO(L,5,15)=-CO(L,5)
      RO(L,5,14)=CO(L,7)
      RO(L,6,16)=-CO(L,6)
      RO(L,6,17)=CO(L,7)
      RO(L,7,1)=-CO(L,7)*CO(L,12)
      RO(L,7,2)=-CO(L,7)*CO(L,12)
      RO(L,7,3)=-CO(L,7)*CO(L,12)
      RO(L,7,13)=-CO(L,7)
      RO(L,7,14)=-CO(L,7)
      RO(L,7,15)=CO(L,5)
      RO(L,7,16)=CO(L,6)
      RO(L,7,17)=-CO(L,7)
      RO(L,7,18)=-CO(L,7)
      RO(L,8,5)=-CO(L,8)
      RO(L,8,6)=CO(L,9)
```

```
      RO(L,8,18)=CO(L,7)
      RO(L,8,19)=-CO(L,8)
      RO(L,8,20)=-CO(L,8)
      RO(L,8,1)=CO(L,7)*CO(L,12)
      RO(L,8,2)=CO(L,7)*CO(L,12)
      RO(L,8,3)=CO(L,7)*CO(L,12)
      RO(L,9,3)=CO(L,7)*CO(L,12)
      RO(L,9,4)=-CO(L,9)
      RO(L,9,5)=CO(L,8)
      RO(L,9,6)=-CO(L,9)
      RO(L,9,7)=CO(L,5)
      RO(L,10,20)=CO(L,8)
      RO(L,11,2)=CO(L,7)*CO(L,12)
      RO(L,12,1)=-CO(L,7)*CO(L,12)
      RO(L,12,2)=-CO(L,7)*CO(L,12)
   50 RO(L,12,3)=-CO(L,7)*CO(L,12)
      DO 5 L=1,12
      R(L,1,1,19)=C(L,1,8)
      R(L,1,1,4)=C(L,1,9)
      R(L,1,1,8)=C(L,1,5)
      R(L,1,1,11)=C(L,1,5)
      R(L,1,1,13)=C(L,1,7)
      R(L,1,2,8)=C(L,1,5)
      R(L,1,2,9)=C(L,1,3)
      R(L,1,2,10)=-C(L,1,2)
      R(L,1,3,9)=-C(L,1,3)
      R(L,1,3,10)=C(L,1,2)
      R(L,1,3,11)=C(L,1,5)
      R(L,1,3,12)=-C(L,1,3)
      R(L,1,3,13)=C(L,1,7)
      R(L,1,4,1)=2.0D0*C(L,1,7)*C(L,1,12)
      R(L,1,4,4)=C(L,1,9)
      R(L,1,4,12)=C(L,1,3)
      R(L,1,4,19)=C(L,1,8)
      R(L,1,5,7)=-C(L,1,5)
      R(L,1,5,8)=-C(L,1,5)
      R(L,1,5,11)=-C(L,1,5)
      R(L,1,5,15)=-C(L,1,5)
      R(L,1,5,14)=C(L,1,7)
      R(L,1,6,16)=-C(L,1,6)
      R(L,1,6,17)=C(L,1,7)
      R(L,1,7,1)=-C(L,1,7)*C(L,1,12)
      R(L,1,7,2)=-C(L,1,7)*C(L,1,12)
      R(L,1,7,3)=-C(L,1,7)*C(L,1,12)
      R(L,1,7,13)=-C(L,1,7)
      R(L,1,7,14)=-C(L,1,7)
      R(L,1,7,15)=C(L,1,5)
      R(L,1,7,16)=C(L,1,6)
      R(L,1,7,17)=-C(L,1,7)
      R(L,1,7,18)=-C(L,1,7)
      R(L,1,8,5)=-C(L,1,8)
      R(L,1,8,6)=C(L,1,9)
      R(L,1,8,18)=C(L,1,7)
      R(L,1,8,19)=-C(L,1,8)
      R(L,1,8,20)=-C(L,1,8)
      R(L,1,8,1)=C(L,1,7)*C(L,1,12)
      R(L,1,8,2)=C(L,1,7)*C(L,1,12)
      R(L,1,8,3)=C(L,1,7)*C(L,1,12)
      R(L,1,9,3)=C(L,1,7)*C(L,1,12)
      R(L,1,9,4)=-C(L,1,9)
      R(L,1,9,5)=C(L,1,8)
```

```
      R(L,1,9,6)=-C(L,1,9)
      R(L,1,9,7)=C(L,1,5)
      R(L,1,10,20)=C(L,1,8)
      R(L,1,11,2)=C(L,1,7)*C(L,1,12)
      R(L,1,12,1)=-C(L,1,7)*C(L,1,12)
      R(L,1,12,2)=-C(L,1,7)*C(L,1,12)
    5 R(L,1,12,3)=-C(L,1,7)*C(L,1,12)
C     NOW PERFORM INTEGRATION BY TRAPEZOID RULE
C     STEP IS 5 SECONDS, ONE STEP
      DO 6 L=1,12
      DO 6 K=1,N
      DO 6 J=1,12
      B=5.0D0*((0.5D0*RO(L,J,K))+(0.5D0*R(L,1,J,K)))
    6 R(L,1,J,K)=B
C     CALC THE ACTUAL MEASURED Y1 VALUE
      DO 7 L=1,12
      DO 7 J=1,12
      Y1(L,1,J)=C(L,1,J)-CO(L,J)
    7 W(L,1,J)=1.0D0/DABS(Y1(L,1,J))
C     CALC RATE CONSTANT FOR EACH TEMP BASED ON 730 F
      T(1)=622.04
      T(2)=633.15
      T(3)=638.71
      T(4)=649.82
      T(5)=655.37
      T(6)=660.93
      T(7)=666.48
      T(8)=672.04
      T(9)=677.59
      T(10)=683.15
      T(11)=688.71
      T(12)=694.26
      DO 60 K=1,20
   60 A(K)=RA(K)*DEXP(P(K)/(1.987D0*660.930))
      DO 70 L=1,12
      DO 70 K=1,20
   70 RG(L,K)=A(K)*DEXP(-1.0D0*P(K)/(1.987D0*T(L)))
      DO 8 L=1,12
      DO 8 J=1,12
      Y2(L,1,J)=0.D0
      DO 8 K=1,N
    8 Y2(L,1,J)=Y2(L,1,J)+(RG(L,K)*R(L,1,J,K))
      COST=0.D0
      DO 9 L=1,12
      DO 9 J=1,12
    9 COST=COST+(((Y1(L,1,J)-Y2(L,1,J))*W(L,1,J))**2)
      RETURN
      END
//
0.0
0.0
0.0
.603
.217
231.15
363.1
8.56
1.22
1.45
6.63
110.6
```

0.0
0.0
0.0
.592
.213
227.05
356.65
8.406
1.207
1.418
6.517
108.67
0.0
0.0
0.0
.587
.211
225.0
353.4
8.33
1.19
1.41
6.46
107.7
0.0
0.0
0.0
.577
.207
221.19
347.45
8.19
1.17
1.38
6.35
105.9
0.00
0.00
0.00
.572
.206
219.50
344.08
8.12
1.16
1.37
6.308
105.05
0.0
0.0
0.0
.567
.204
217.51
341.67
8.05
1.15
1.36
6.24
104.10
0.0

0.0
0.0
.562
.202
215.72
338.9
7.98
1.14
1.35
6.19
103.2
0.0
0.0
0.0
.558
.201
213.95
336.1
7.92
1.13
1.34
6.14
102.4
0.0
0.0
0.0
.553
.199
212.06
333.1
7.85
1.12
1.33
6.08
101.5
0.0
0.0
0.0
.549
.197
210.51
330.7
7.79
1.11
1.32
6.04
100.7
0.0
0.0
0.0
.544
.196
208.67
327.79
7.72
1.10
1.31
5.99
99.9
0.0
0.0

0.0
.54
.194
207.17
325.4
7.67
1.09
1.30
5.94
99.2
37.08
14.19
4.28
71.03
48.33
242.36
118.90
6.76
18.10
17.69
20.98
78.41
54.68
23.89
6.39
79.99
54.64
246.93
100.65
7.46
26.81
19.06
24.06
75.36
118.69
41.78
10.74
105.17
51.22
210.90
73.16
8.45
37.64
25.35
18.21
41.76
159.05
47.06
13.82
123.23
57.85
194.77
36.29
7.63
43.76
27.23
20.53
33.53
181.49
65.81
16.12

108.25
48.32
168.26
27.59
6.01
41.97
31.09
17.06
33.13
115.28
45.15
10.50
102.13
50.67
186.63
42.79
6.04
44.61
30.67
19.04
49.52
241.43
53.14
12.05
113.35
44.73
171.80
29.76
6.40
54.72
39.59
17.16
24.50
118.10
40.04
7.68
82.77
32.43
187.4
79.30
6.19
42.98
29.66
16.10
48.87
161.20
37.66
8.09
83.67
34.47
189.40
70.00
6.0
44.23
37.55
17.20
53.37
192.75
29.65
6.78
84.84

```
38.28
146.96
28.05
6.0
55.19
44.85
20.52
40.58
266.0
46.07
7.98
127.89
18.97
154.61
67.58
6.0
39.95
48.53
19.29
23.41
158.14
16.00
4.15
77.66
24.56
167.70
87.86
6.0
36.14
39.93
17.19
44.72
25.21
20.80
     7.172D-3
   3.162D-20
2.906
0.7875
0.2403
     2.79D-17
13.67
3.089
   5.153D-18
.07805
.07566
.07163
   1.143D-17
.09225
.07692
.08373
2.0228
1.1645
//
```

PROGRAM KINT730

```
      EXTERNAL FEX,JEX
      DOUBLE PRECISION ATOL,RWORK,RTOL,T,TOUT,Y
      DIMENSION Y(12),RWORK(212),IWORK(20)
      NEQ=12
C     730 F INITIAL CONDITIONS
      Y(1)=0.D0
      Y(2)=0.D0
      Y(3)=0.D0
      Y(4)=0.567D-5
      Y(5)=0.204D-5
      Y(6)=217.51D-5
      Y(7)=341.67D-5
      Y(8)=8.05D-5
      Y(9)=1.150D-5
      Y(10)=1.36D-5
      Y(11)=6.240D-5
      Y(12)=104.1D-5
      T=0.D0
      TOUT=.50D0
      ITOL=1
      RTOL=1.D-15
      ATOL=1.D-15
      ITASK=1
      ISTATE=1
      IOPT=0
      LRW=212
      LIW=20
      MF=10
      DO 100 IOUT=1,10
    5 CALL LSODE(FEX,NEQ,Y,T,TOUT,ITOL,RTOL,ATOL,ITASK,ISTATE,IOPT,
     1RWORK,LRW,IWORK,LIW,JEX,MF)
      DO 101 J=1,12
      WRITE(6,25)T,J,Y(J)
   25 FORMAT(5X,3HT= ,F10.5,5X,4HY   ,I2,3H   ,D13.4)
  101 CONTINUE
      IF(ISTATE.LT. 0)GO TO 80
  100 TOUT=TOUT+.50
      WRITE(6,60)IWORK(11),IWORK(12),IWORK(13)
   60 FORMAT(/12H NO. STLPS =,I4,11H  NO. F-S =,I4,11H  NO. J-S =,I4)
      STOP
   80 WRITE(6,90)ISTATE
   90 FORMAT(///22H ERROR HALT.. ISTATE =,I3)
      STOP
      END
      SUBROUTINE FEX(NEQ,T,Y,YDOT)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION Y(12),YDOT(12)
C     INSERT EQUATIONS
      YDOT(1)=2.0228D0*Y(8)+3.162D-21*Y(9)+3.3053D-17*Y(5)+7.566D-2*Y(7)
      YDOT(2)=0.279D-16*Y(5)+13.67D0*Y(3)-3.089D0*Y(2)
      YDOT(3)=-13.748D0*Y(3)+3.089D0*Y(2)+7.566D-2*Y(7)+0.5153D-17*Y(5)
      YDOT(4)=-.3162D-20*Y(9)+50.42D0*Y(7)*Y(12)+7.566D-2*Y(3)+2.0228D0*Y
     &(8)
      YDOT(5)=0.07163D0*Y(7)-0.2403D0*Y(5)
      YDOT(6)=0.07692D0*Y(7)-0.09225D0*Y(6)
      YDOT(7)=-.1143D-16*Y(5)+.09225D0*Y(6)-.30794D0*Y(7)-46.02*Y(7)*Y(12
     &)
      YDOT(8)=-.7875D0*Y(9)+.08373D0*Y(7)-6.0933D0*Y(8)+46.02D0*Y(7)*Y(12
     &)
      YDOT(9)=2.906D0*Y(8)+.2403D0*Y(5)+.007172D0*Y(7)*Y(12)-.7875D0*Y(9
     &)
      YDOT(10)=1.1645D0*Y(8)
```

```
      YDOT(11) =20.80D0*Y(7)*Y(12)
      YDOT(12) =-46.02D0*Y(7)*Y(12)
      RETURN
      END
      SUBROUTINE JEX(NEQ,T,Y,ML,MU,PD,NRPD)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION Y(11),PD(NRPD,11)
      RETURN
      END
```

Constant, William David, B.S. Louisiana State University, 1977
M.S., Louisiana State University, 1980
Doctor of Philosophy, Summer Commencement, 1984
Major: Chemical Engineering; Minor: Petroleum Engineering
Hydrocracking of Model Coal Derived Liquid Components Over a Zeolite Catalyst
Dissertation directed by Professor Edward McLaughlin
Pages in Dissertation, 444. Words in Abstract, 345.

ABSTRACT

Hydrocracking of fluorene was investigated over a nickel loaded Y zeolite in a fixed bed flow reactor using decalin as a donor solvent. This system served as a model for typical commercial donor solvent operations in order to develop a representative kinetic model and propose a reaction mechanism for refining of coal derived liquids.

After performing a qualitative investigation, base operating conditions of 661°K, 14.8 bar total pressure, 20 weight percent fluorene in decalin and a hydrogen to hydrocarbon ratio of 42 at a space-time of 4.8 seconds were established for the process. For each experimental series, the variable of interest was adjusted maintaining other conditions constant. Over the range of variables investigated, the effects of space-time and temperature were found to be most significant. No thermal reactions were observed during the study. The effect of hydrogen pressure was studied from 8.2 to 35.8 bar at 661°K, and no significant changes in the reaction occurred. Deactivation and coking were significant and the coke formation was found to be a function of catalyst exposure time. Deactivation was not included in the kinetic model as the route of coke formation was unknown.

Two kinetic models were developed using pseudo-homogeneous rate expressions of the chemistry as understood at this time. Rate

coefficients were determined by numerical analysis of the experimental data and activation energies estimated. An overall reaction mechanism was proposed taking into account the roles of the donor solvent, catalyst, and hydrogen. It was proposed that decalin transferred hydrogen to fluorene adsorbed on the catalyst in a reactive state. The cis-decalin isomer was highly reactive in isomerization, dehydrogenation, and cracking while trans-decalin was not as reactive. The kinetic model incorporates three routes for cracking of fluorene after partial hydrogenation from decalin; the side ring, the phenyl-methyl bond of the central ring, and both sides of the central ring.

Each component, decalin, nickel on the acidic catalyst, and hydrogen were found essential for hydrocracking of fluorene to occur. The product distribution was primarily benzenes, cyclopentanes, and C_2-C_6 hydrocarbon gases.

VITA

William David Constant, the son of Montez H. and Warren L. Constant, was born in Bunkie, Louisiana, on May 15, 1954. He attended Bunkie Elementary and Bunkie High School, from which he graduated in May, 1972. From August, 1972 to May, 1974, he continued his education at Louisiana State University at Alexandria and then transferred to Louisiana State University at Baton Rouge, from which he graduated in May, 1977, receiving a Bachelor of Science degree in Chemical Engineering.

Upon graduation, he was employed as a Chemical Engineer at Ethyl Corporation in Baton Rouge until he returned to LSU to begin graduate studies in August, 1978 on an Exxon Fellowship. In December, 1980, he received his Master of Science degree in Chemical Engineering. During his graduate studies, he was an instructor in the Department of Chemical Engineering at LSU, teaching courses in material balances and transport sciences.

The author is a member of Tau Beta Pi, Phi Lambda Upsilon, Gamma Beta Phi, The American Institute of Chemical Engineers, The Society of Petroleum Engineers, and The American Chemical Society. He is married to the former Susan Averett of New Orleans, Louisiana, and they reside in Baton Rouge.

EXAMINATION AND THESIS REPORT

Candidate: William David Constant

Major Field: Chemical Engineering

Title of Thesis: Hydrocracking of Model Coal Derived Liquid Components Over a Zeolite Catalyst

Approved:

Major Professor and Chairman

Dean of the Graduate School

EXAMINING COMMITTEE:

Date of Examination:

July 13, 1984